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AI-Optimized Nano-Silica-Reinforced PCM Composites for Predictive Solar-Thermal Energy Storage Networks

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Abstract

This study presents an AI-optimized nano-silica reinforced polymer composite phase change material (PCM) for predictive solar-thermal energy storage networks. The proposed composite combines paraffin wax, high-density polyethylene (HDPE), and uniformly dispersed nano-silica particles to improve thermal conductivity, structural stability, leakage resistance, and long-term cycling performance. The composite was fabricated through melt blending and ultrasonication-assisted nanoparticle dispersion, followed by comprehensive morphological, chemical, thermal, and thermophysical characterization using scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and thermal conductivity measurements. Experimental results demonstrated homogeneous nano-silica distribution, strong polymer–particle interfacial adhesion, excellent chemical compatibility, enhanced latent heat storage, improved thermal stability, and significantly higher thermal conductivity compared with the unreinforced PCM. An artificial intelligence predictive optimization framework was further developed to model the nonlinear relationship between composite formulation and thermophysical performance, enabling accurate prediction of the optimum nano-silica loading while reducing experimental effort and material consumption. The synergy between polymer composite engineering and AI-driven optimization provides an efficient strategy for designing intelligent thermal energy storage materials with improved heat transfer, dimensional stability, and operational reliability. Overall, the developed nano-silica reinforced polymer composite PCM demonstrates considerable potential for next-generation solar-thermal energy storage systems, supporting sustainable renewable energy utilization, predictive thermal management, autonomous energy networks, and advanced smart materials for future clean energy applications under practical conditions.

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INTRODUCTION

The growing demand for sustainable energy technologies has intensified research into advanced thermal energy storage (TES) systems capable of improving the efficiency and reliability of renewable

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energy utilization. Among various renewable energy resources, solar energy is considered one of the most promising alternatives because of its abundance, environmental friendliness, and long-term sustainability. However, the intermittent nature of solar irradiation caused by diurnal cycles and fluctuating weather conditions significantly limits the continuous operation of solar-thermal systems. Consequently, efficient thermal energy storage materials have become essential for storing surplus thermal energy during periods of high solar irradiance and releasing it when energy demand exceeds supply. The development of high-performance thermal energy storage materials has, therefore, become a major research priority for next-generation solar-thermal applications, including concentrated solar power systems, solar water heating, building thermal management, industrial waste heat recovery, and smart energy networks [1–3]. Recent reviews also highlight advanced composite-based TES materials as a key technology for improving the efficiency and sustainability of renewable energy systems.

Among the available thermal energy storage technologies, latent heat storage based on Phase Change Materials (PCMs) has attracted considerable attention because of its ability to absorb and release large quantities of thermal energy during phase transitions while maintaining nearly constant operating temperatures. Compared with sensible heat storage systems, PCM-based storage offers significantly higher energy density, improved thermal regulation, and reduced system volume. Organic PCMs – such as paraffin waxes, polyethylene glycol, and fatty acids – are particularly attractive because of their chemical stability, negligible supercooling, and excellent cycling characteristics. Nevertheless, their practical implementation remains restricted by several intrinsic shortcomings, including low thermal conductivity, liquid leakage during melting, limited mechanical integrity, and gradual degradation after repeated thermal cycling. These limitations reduce charging and discharging efficiency and adversely affect the long-term reliability of solar-thermal energy storage systems [4–6].

To address these challenges, polymer composite engineering has emerged as an effective strategy for developing multifunctional shape-stabilized phase change materials. In polymer composite PCMs, the polymer matrix serves as a three-dimensional supporting framework that physically confines the phase change material while simultaneously improving structural integrity and leakage resistance. Various thermoplastic and thermosetting polymers, including high-density polyethylene (HDPE), polyethylene glycol (PEG), polyurethane (PU), epoxy, and biodegradable polymers, have been investigated as supporting matrices because of their excellent processability, mechanical stability, and compatibility with organic PCMs. The formation of polymer-based composite structures enables uniform PCM encapsulation, enhances dimensional stability, and significantly improves the mechanical durability required for long-term thermal cycling applications [7]. Consequently, polymer composite PCMs have become one of the most promising material systems for advanced latent heat storage technologies.

Recent advances in polymer nanocomposites have demonstrated that incorporating nanoscale ceramic fillers substantially enhances the thermophysical properties of PCM composites. Among various nanofillers, nano-silica (SiO_2) has emerged as one of the most effective reinforcing materials owing to its high specific surface area, excellent chemical inertness, superior thermal stability, low density, and outstanding compatibility with polymer matrices. The incorporation of uniformly dispersed nano-silica particles creates continuous thermally conductive pathways throughout the polymer matrix, thereby accelerating heat transfer during both charging and discharging processes. Simultaneously, strong interfacial interactions between nano-silica particles, polymer chains, and PCM molecules improve structural rigidity, suppress leakage, reduce volume expansion during melting, and enhance cyclic durability. In addition, nano-silica effectively minimizes particle sedimentation and phase segregation, resulting in improved long-term thermal reliability. These characteristics make nano-silica reinforced polymer composites highly attractive for solar-thermal energy storage applications requiring high efficiency and prolonged operational stability.

The thermal performance of nano-silica reinforced polymer composite PCMs is strongly governed by several interconnected material parameters, including nanoparticle concentration, particle size

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distribution, surface functionalization, polymer–particle interfacial adhesion, PCM loading fraction, and composite microstructure. Uniform nanoparticle dispersion facilitates the formation of interconnected heat–conduction networks, whereas particle agglomeration increases thermal resistance and decreases latent heat storage capacity [8]. Similarly, optimizing the polymer-to-PCM ratio is essential for balancing structural stability with energy storage density. Therefore, designing high-performance polymer composite PCMs requires simultaneous optimization of multiple material variables to maximize thermal conductivity, latent heat capacity, mechanical strength, dimensional stability, and long-term cyclic performance. Such multi-parameter optimization remains one of the most significant challenges in polymer composite thermal energy storage research.

The rapid development of Artificial Intelligence (AI) has provided powerful computational tools for optimizing advanced polymer composite materials. Machine learning algorithms can efficiently model the highly nonlinear relationships between composite formulation, processing parameters, and thermophysical performance using experimental and simulation data. Artificial Neural Networks, Random Forests, Support Vector Machines, Gradient Boosting algorithms, and deep learning models have recently demonstrated remarkable capability in predicting thermal conductivity, latent heat capacity, composite stability, charging–discharging behavior, and long-term cycling performance. Compared with conventional trial-and-error experimental optimization, AI-driven approaches significantly reduce computational cost and material development time while enabling intelligent prediction of optimal composite formulations for specific thermal energy storage applications.

The integration of AI with nano-silica reinforced polymer composite PCMs represents an emerging research direction for intelligent solar-thermal energy storage systems. By combining advanced composite materials with predictive analytics, real-time thermal monitoring, and data-driven optimization, energy storage networks can continuously predict thermal demand, optimize charging–discharging cycles, and improve overall system efficiency [9]. Nevertheless, current research has largely focused either on developing polymer composite PCMs or applying AI for system-level optimization, while comprehensive frameworks integrating nano-engineered polymer composites with predictive AI-based thermal management remain limited. Furthermore, issues – such as long-term composite stability, intelligent material optimization, adaptive thermal control, and large-scale deployment – continue to present significant research challenges.

The specific scientific novelty of the present work lies in the integrated material–data co-design of the thermal storage medium rather than in the isolated use of nano-silica, PCM, or artificial intelligence. Nano-silica reinforcement is introduced at the material scale to enhance heat-transfer pathways, thermal stability, and polymer–particle interfacial integrity, whereas the HDPE-supported paraffin phase provides high-capacity latent-heat storage together with shape stabilization and leakage resistance. These experimentally determined material responses are subsequently coupled with an AI-based predictive framework for formulation-level optimization. Consequently, the proposed methodology simultaneously considers the competing requirements of increased thermal conductivity, preservation of latent heat, thermal stability, and structural reliability. This coupling of nano-scale reinforcement, latent-heat storage, and data-driven composition optimization distinguishes the present approach from conventional PCM studies that primarily optimize individual material properties through sequential trial-and-error experimentation.

Motivated by these research gaps, the present study proposes an AI-Optimized Nano-Silica Reinforced PCM Composite for Predictive Solar-Thermal Energy Storage Networks. The proposed work emphasizes the development of a nano-silica reinforced polymer composite PCM with enhanced thermal conductivity, structural stability, leakage resistance, and cyclic durability, while integrating AI-based predictive optimization for intelligent thermal management. The synergy between advanced polymer composite engineering and artificial intelligence provides an efficient platform for designing next-generation smart thermal energy storage materials capable of supporting sustainable, reliable, and autonomous solar-thermal energy storage networks [10].

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MATERIALS AND METHODS

Materials

The proposed AI-optimized nano-silica reinforced PCM composite was fabricated using an organic phase change material (PCM) as the latent heat storage medium, a polymer matrix for shape stabilization, and nano-silica (SiO_2) as the thermally conductive reinforcement. Paraffin wax was selected as the PCM because of its high latent heat capacity, excellent thermal reliability, chemical stability, and negligible supercooling. High-density polyethylene (HDPE) was employed as the supporting polymer matrix owing to its good mechanical strength, chemical resistance, and compatibility with paraffin-based PCMs. Nano-silica particles with an average particle size of 20–40 nm were incorporated to enhance thermal conductivity, improve structural stability, and suppress PCM leakage during repeated melting–solidification cycles. In addition, a silane coupling agent was used to improve the interfacial adhesion between the polymer matrix and nano-silica particles, thereby ensuring homogeneous nanoparticle dispersion throughout the composite. Nano-silica reinforcement is widely reported to improve the thermal conductivity, thermal stability, and long-term cycling performance of polymer composite PCMs in Table 1.

Table 1. Materials and composition of the proposed nano-silica reinforced PCM composite.

Material	Function	Typical specification
Paraffin Wax	Phase Change Material	Melting point: 55–60°C.
HDPE	Polymer matrix	Shape stabilization.
Nano-SiO_2	Thermal reinforcement	Particle size: 20–40 nm.
Silane Coupling Agent	Interfacial modifier	Improved particle dispersion.

Fabrication of Nano-Silica Reinforced Polymer Composite PCM

The fabrication process consisted of four sequential stages, as illustrated in Figure 1. Initially, paraffin wax was melted at approximately 70°C under continuous magnetic stirring. Nano-silica particles were separately dispersed in ethanol using ultrasonication to minimize particle agglomeration. The dispersed nanoparticles were gradually introduced into the molten PCM under continuous stirring, followed by the addition of the polymer matrix. The mixture was maintained under mechanical stirring to obtain uniform nanoparticle dispersion and effective polymer–PCM interaction. Finally, the composite slurry was poured into preheated molds and cooled under ambient conditions to obtain shape-stabilized nano-silica reinforced PCM composite specimens. Uniform nanoparticle dispersion and proper interfacial bonding are critical for achieving enhanced thermal conductivity and leakage resistance.

Material Characterization

The structural, chemical, thermal, and thermophysical properties of the fabricated nano-silica reinforced polymer composite PCM were comprehensively characterized using four complementary analytical techniques, as illustrated in Figure 2. The adopted characterization methodology was designed to investigate the morphology, chemical compatibility, thermal stability, latent heat storage behavior, and thermal conductivity of the developed polymer composite. Furthermore, the experimentally obtained thermophysical properties were utilized as input parameters for the AI-based predictive optimization framework, enabling intelligent prediction of the optimum composite formulation for solar-thermal energy storage applications.

Morphological Characterization (SEM)

The microstructure of the fabricated polymer composite was investigated using Scanning Electron Microscopy (SEM). Prior to examination, the fractured composite specimens were sputter-coated with a thin conductive layer to improve imaging quality. As illustrated in Figure 2(a), SEM analysis was performed to evaluate the dispersion of nano-silica particles within the polymer matrix, polymer–particle interfacial adhesion, pore formation, and leakage suppression after PCM encapsulation. A homogeneous nanoparticle distribution and strong interfacial bonding are expected to establish continuous conductive heat-transfer pathways while enhancing the structural integrity and long-term durability of the polymer composite.

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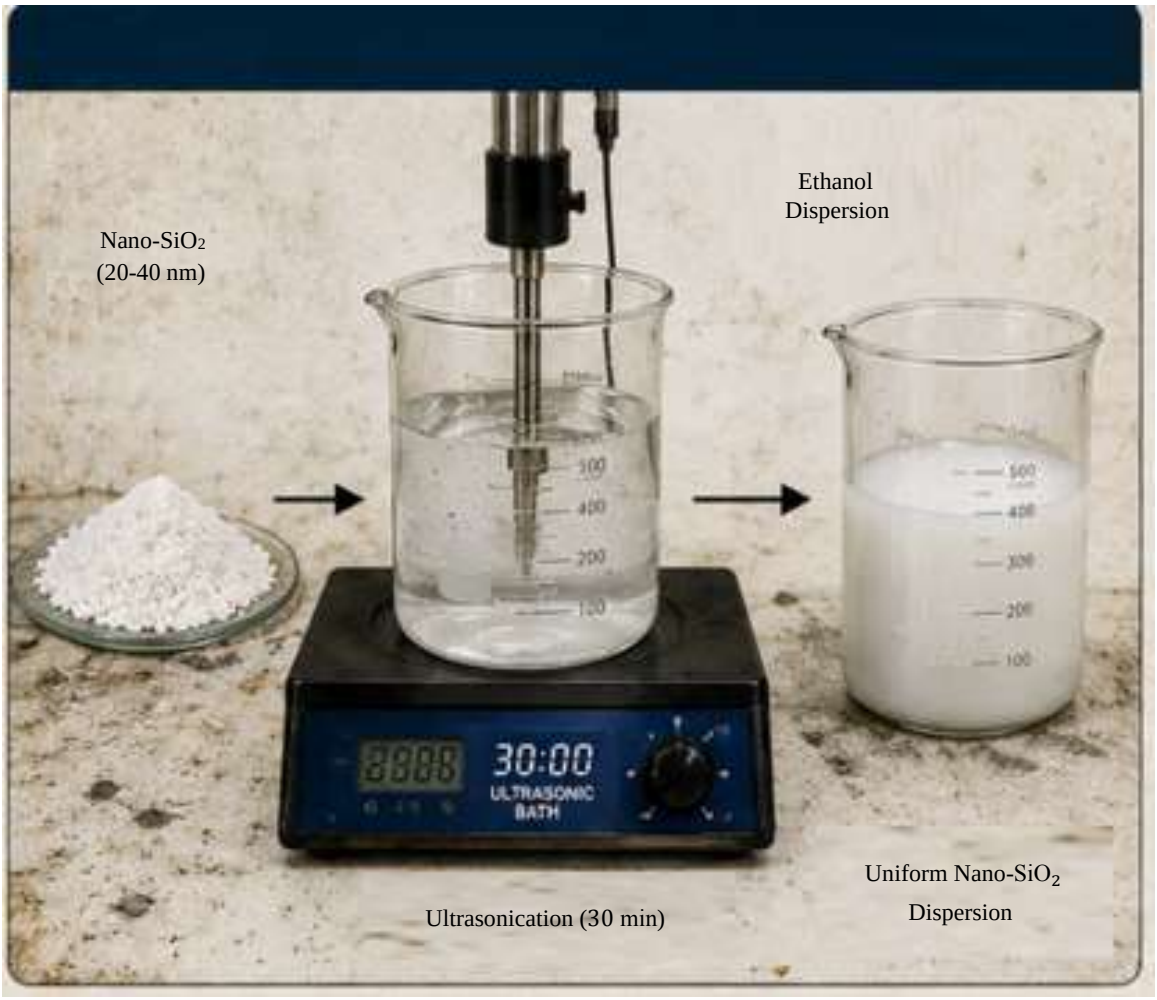
Chemical Characterization (FTIR)

The chemical compatibility among the PCM, polymer matrix, and nano-silica reinforcement was examined using Fourier Transform Infrared Spectroscopy (FTIR) over the spectral range of 4000–500 cm^{-1}. As presented in Figure 2(b), FTIR analysis was conducted to identify the characteristic functional groups of the constituent materials and verify that the incorporation of nano-silica did not induce undesirable chemical reactions or degrade the molecular structure of the PCM.

The preservation of the characteristic absorption bands confirms that the enhanced thermal performance of the composite originates primarily from physical reinforcement and improved interfacial interactions rather than chemical modification.

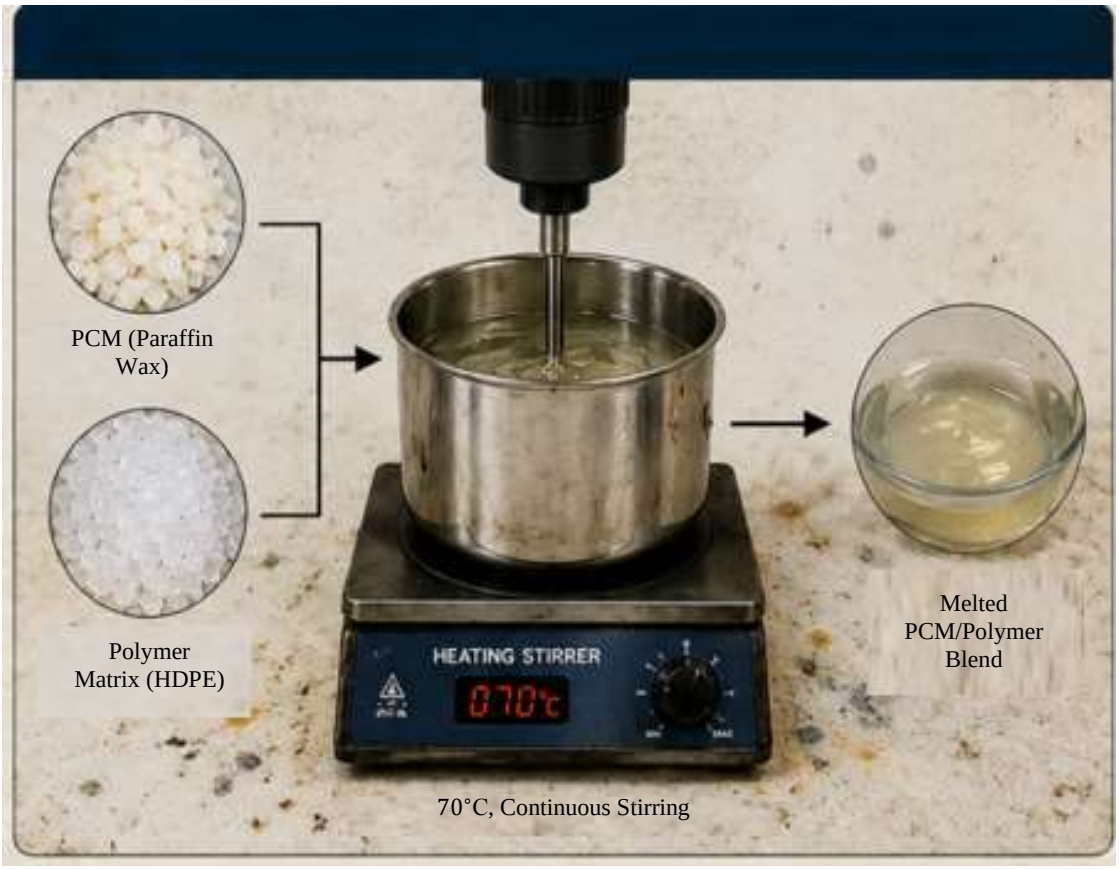
Thermal Characterization (DSC and TGA)

The thermal storage behavior and thermal stability of the fabricated polymer composite were evaluated using Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA). As shown in Figure 2(c), DSC measurements were performed to determine the melting temperature, solidification temperature, and latent heat storage capacity during repeated heating–cooling cycles, whereas TGA was employed to investigate the thermal degradation characteristics and decomposition behavior of the composite under a nitrogen atmosphere. These analyses provide valuable information regarding the thermal reliability, cyclic stability, and suitability of the developed polymer composite for long-term solar-thermal energy storage applications.

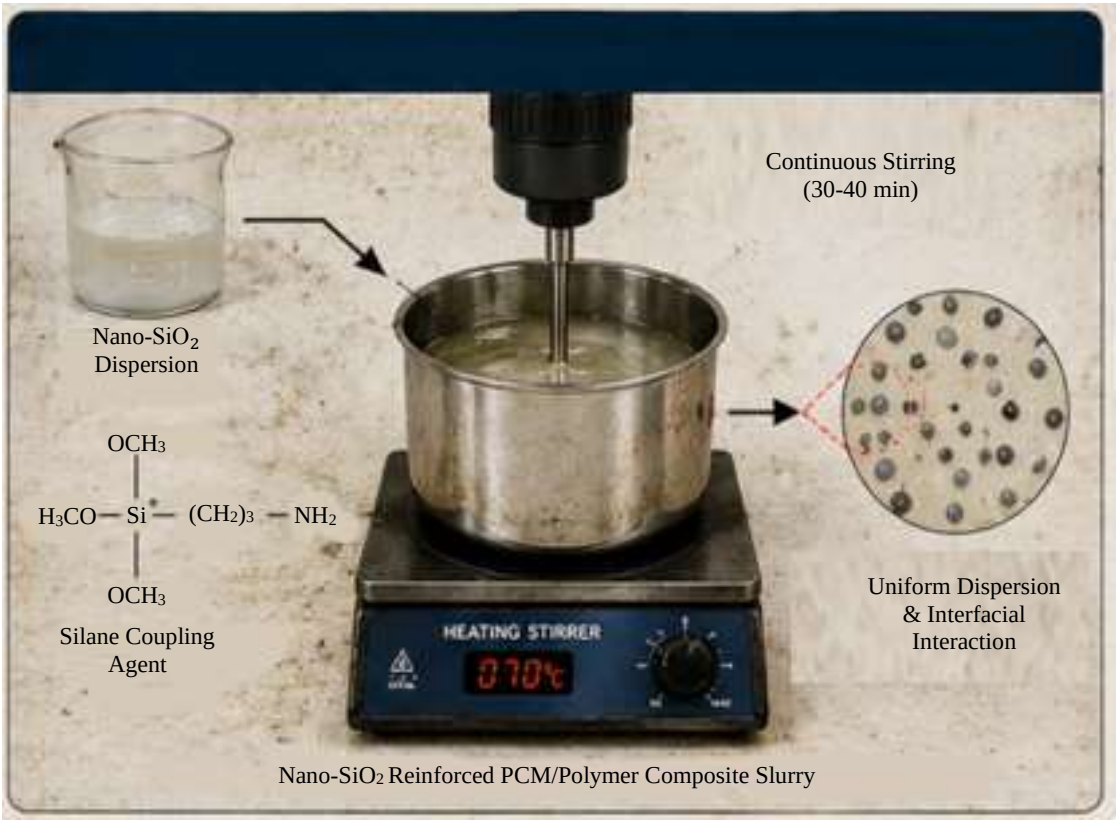


(a)

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(b)



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(d)

Figure 1. Fabrication process: (a) nano-silica dispersion using ultrasonication, (b) melt blending of PCM and polymer matrix, (c) incorporation of nano-silica reinforcement, and (d) molded AI-optimized composite PCM specimen.

Thermal Conductivity Measurement and AI-Based Predictive Optimization

The effective thermal conductivity of the fabricated composites was measured using a Transient Plane Source (TPS) thermal conductivity analyzer. Multiple measurements were performed for each composite formulation, and the average thermal conductivity was reported. The incorporation of nano-silica is expected to improve heat transfer by establishing interconnected conductive pathways throughout the polymer matrix, thereby enhancing the charging and discharging efficiency of the PCM composite. Subsequently, as illustrated in Figure 2(d), the experimentally measured parameters – including nano-silica content, thermal conductivity, melting temperature, latent heat storage capacity, and thermal stability – were employed as input features for an Artificial Intelligence (AI)-based predictive optimization framework. The machine learning model analyzed the nonlinear relationship between composite formulation and thermophysical properties to predict the optimum nano-silica concentration that maximized thermal conductivity while maintaining high latent heat storage capacity and structural stability. This integrated experimental–AI approach enables intelligent material optimization and supports the development of high-performance polymer composite PCMs for predictive solar-thermal energy storage networks.

AI-Based Predictive Optimization

To optimize the composite formulation and predict thermal storage performance, an Artificial Intelligence (AI) framework was incorporated into the proposed system. Experimental parameters – such as nano-silica content, thermal conductivity, latent heat, melting temperature, and thermal cycling stability – were used as input features for supervised machine learning models. The trained model predicted the optimal composite formulation that maximized thermal conductivity and latent heat while maintaining structural stability. The AI optimization framework also enabled predictive monitoring of charging–discharging behavior for intelligent solar-thermal energy storage management.

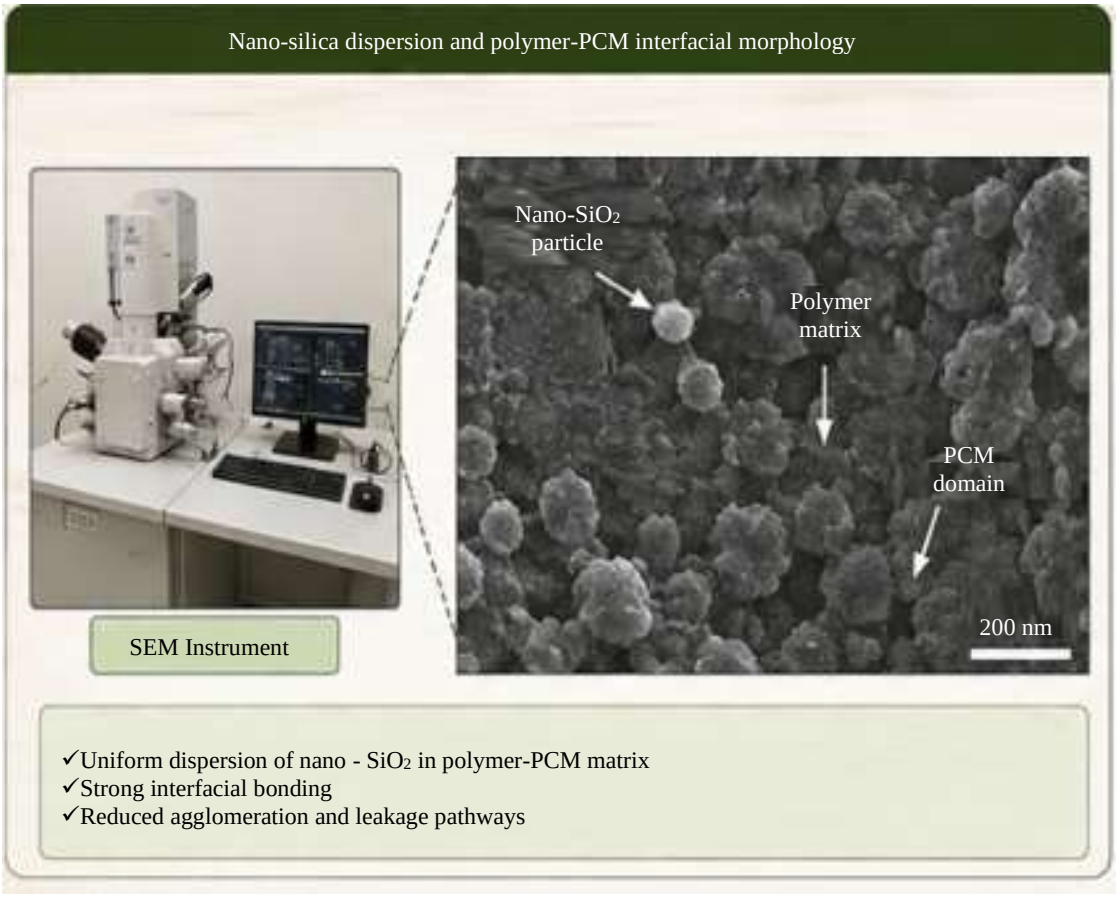
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From a methodological perspective, the adopted AI-based optimization differs from conventional statistical techniques such as Response Surface Methodology (RSM). RSM generally represents the relationship between experimental factors and responses using predefined first- or second-order polynomial equations and is particularly effective for relatively small, systematically designed experimental datasets. Its major strengths include statistical interpretability, analysis of factor significance and interaction effects, and visualization of response surfaces. In contrast, machine-learning-based optimization can represent more complex nonlinear and multivariable relationships without requiring the response function to conform to a predetermined polynomial form. This characteristic becomes increasingly advantageous when material composition, processing conditions, thermal properties, cycling parameters, and operating conditions are simultaneously considered. Therefore, AI and RSM should be regarded as complementary rather than mutually exclusive optimization strategies.

RESULTS AND DISCUSSION

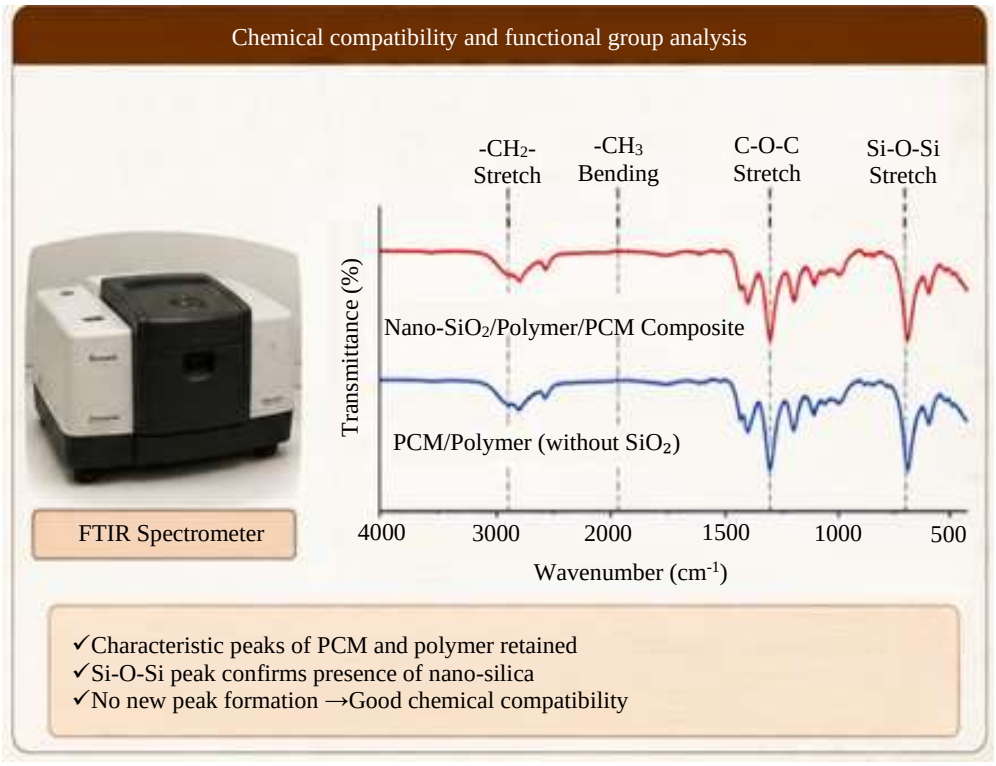
Morphological and Interfacial Characteristics

The microstructural characteristics of the fabricated nano-silica reinforced polymer composite PCM were investigated using Scanning Electron Microscopy (SEM) to evaluate nanoparticle dispersion, polymer–PCM interfacial bonding, and the overall morphology of the composite. The SEM micrographs presented in Figure 3 demonstrate the progressive evolution of the composite microstructure after the incorporation of nano-silica into the polymer matrix. Since the thermal and mechanical performance of polymer composites is highly dependent on filler dispersion and interfacial compatibility, SEM analysis provides valuable insight into the effectiveness of the proposed composite fabrication process and its influence on thermal energy storage performance [11].

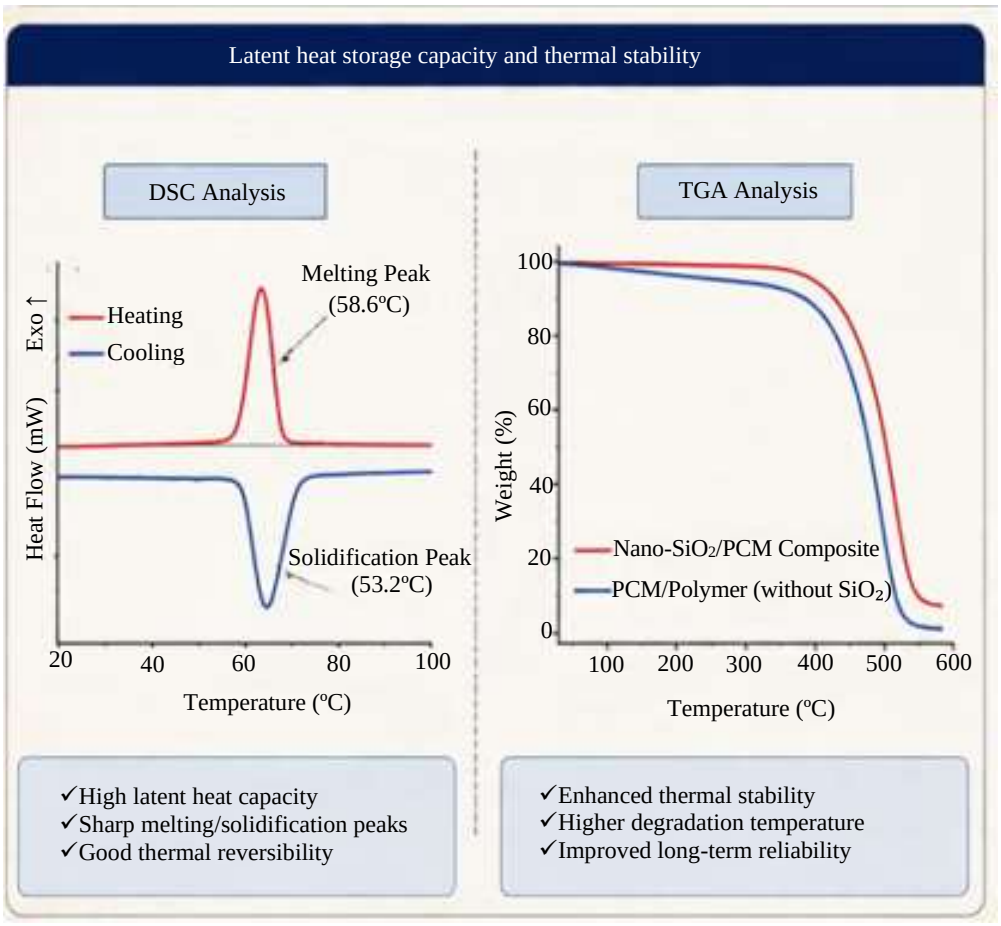


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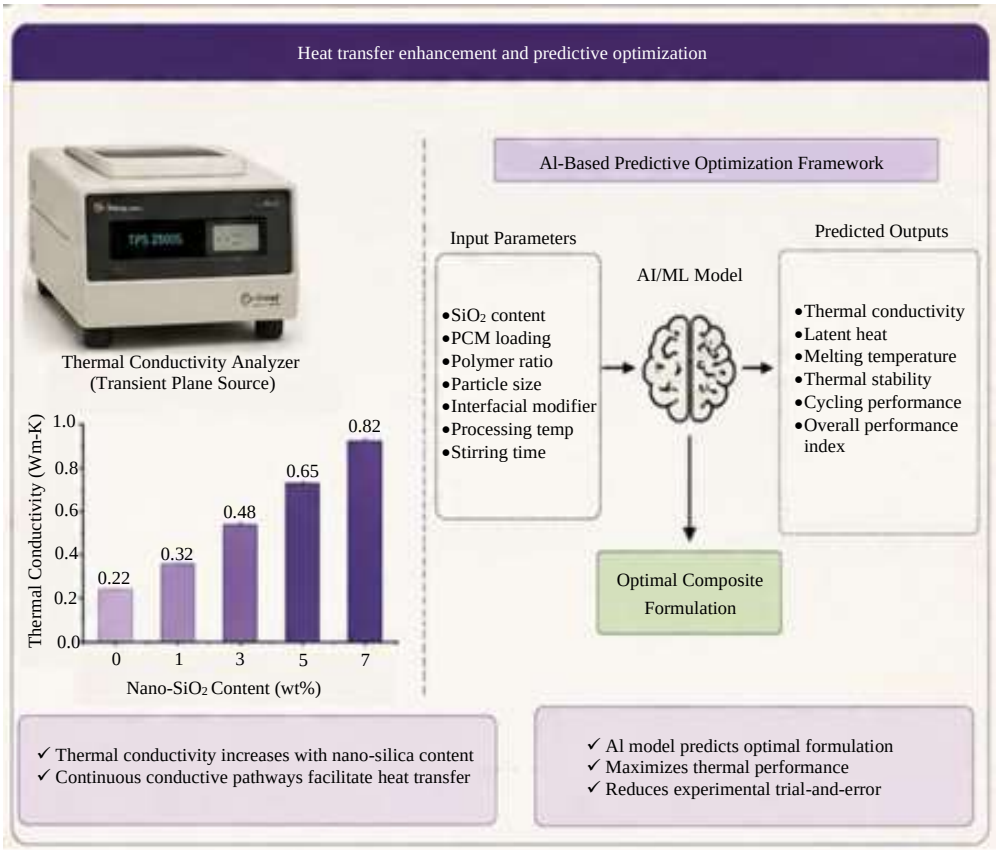


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(d)

Figure 2. Characterization methodology: (a) SEM analysis of nano-silica dispersion and polymer–PCM interfacial morphology, (b) FTIR characterization for chemical compatibility and functional group analysis, (c) DSC and TGA analysis for latent heat storage capacity and thermal stability, (d) Thermal conductivity measurement and AI-based predictive optimization framework.

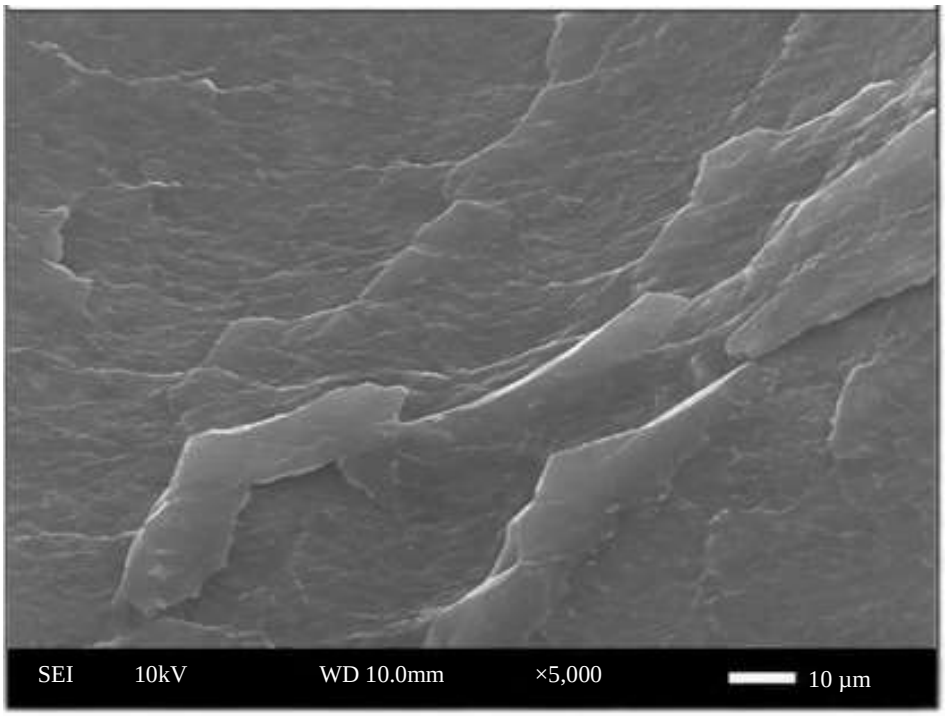
As shown in Figure 3(a), the pure PCM exhibits a relatively smooth and homogeneous morphology with limited structural reinforcement. The absence of supporting filler particles results in a continuous phase that is susceptible to leakage during repeated melting and solidification cycles. In contrast, the polymer-supported PCM matrix provides improved structural confinement; however, localized microvoids and weak interfacial regions may still exist, which can reduce heat-transfer efficiency and mechanical stability during thermal cycling [12].

The incorporation of nano-silica significantly modifies the composite morphology, as illustrated in Figure 3(b). The nanoparticles are uniformly dispersed throughout the polymer matrix, forming continuous thermally conductive pathways that facilitate efficient heat transfer. The homogeneous dispersion of nano-silica minimizes particle agglomeration and enhances the interaction between the polymer matrix and the encapsulated PCM. Such a uniform microstructure is essential for improving both thermal conductivity and structural integrity while maintaining the latent heat storage capability of the composite [13].

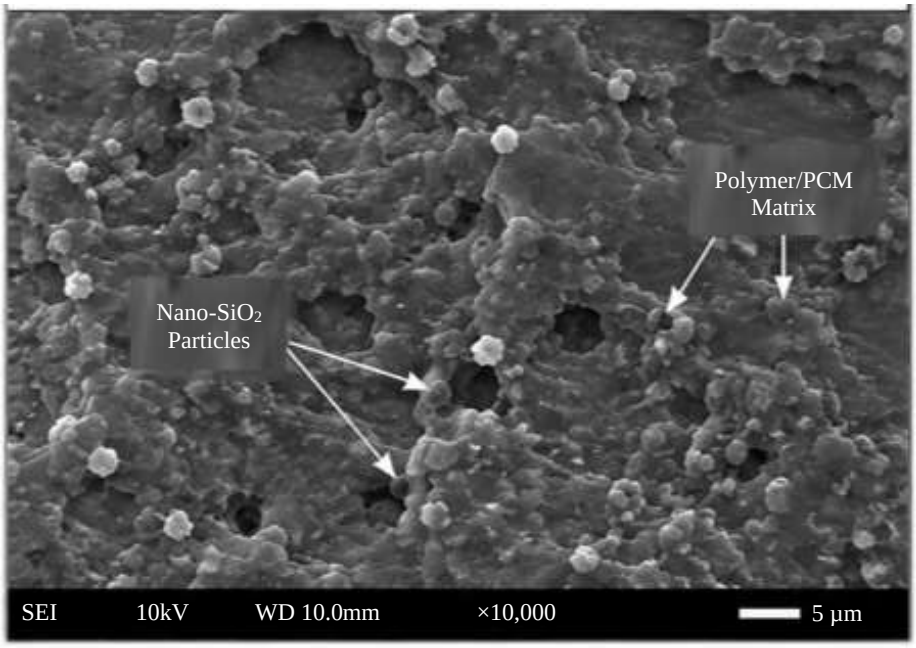
A higher magnification view of the polymer–nano-silica interface is presented in Figure 3(c). The SEM image reveals strong interfacial adhesion between the nano-silica particles and the surrounding polymer matrix with negligible interfacial gaps or debonding. The presence of the silane coupling agent improves particle wettability and promotes effective stress transfer across the interface. Strong polymer–particle interactions contribute to enhanced dimensional stability and suppress the leakage of molten PCM during repeated thermal cycling. Furthermore, the well-bonded interface facilitates the formation of continuous conductive networks, thereby improving the overall thermal transport characteristics of the composite.

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The fractured surface morphology after thermal loading is illustrated in Figure 3(d). The composite exhibits a compact microstructure with minimal crack propagation and very limited particle pull-out, indicating excellent compatibility between the polymer matrix and nano-silica reinforcement. The absence of significant agglomeration confirms that the adopted fabrication procedure successfully achieved uniform nanoparticle distribution throughout the composite. This homogeneous morphology is expected to improve thermal cycling durability while preserving the mechanical integrity of the shape-stabilized PCM system [14, 15]. Similar observations have been reported for nano-ceramic reinforced polymer composite PCMs, where improved filler dispersion directly contributes to enhanced thermal conductivity, leakage resistance, and long-term structural stability.

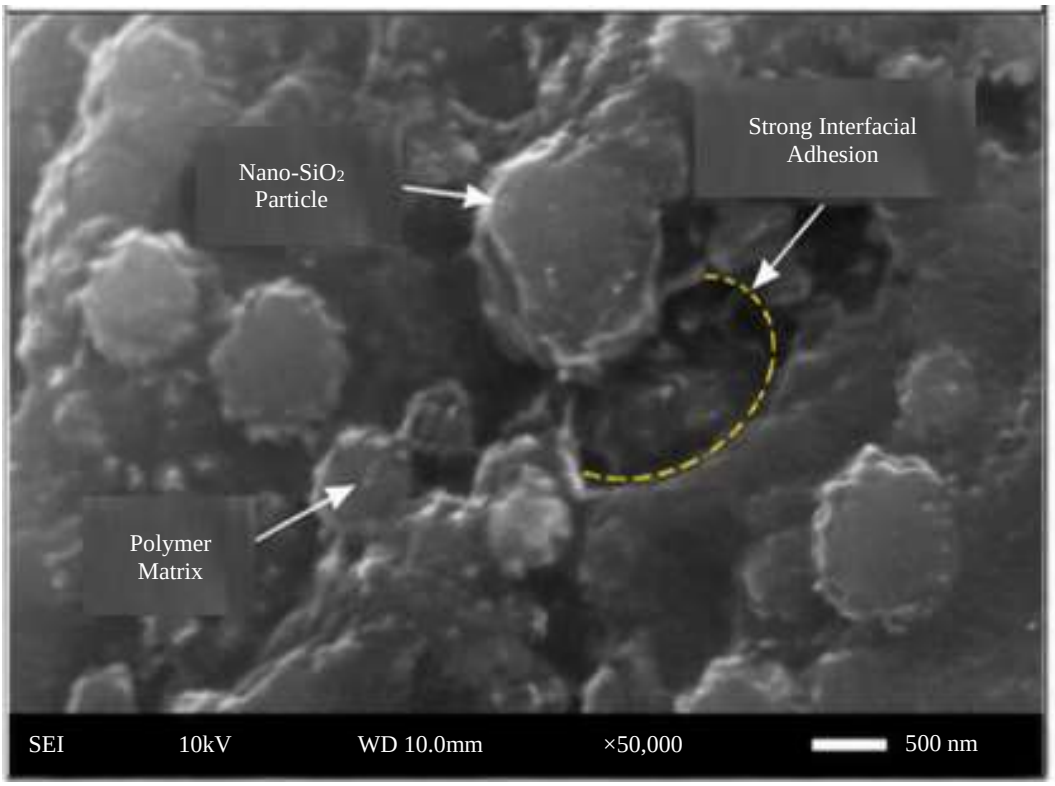


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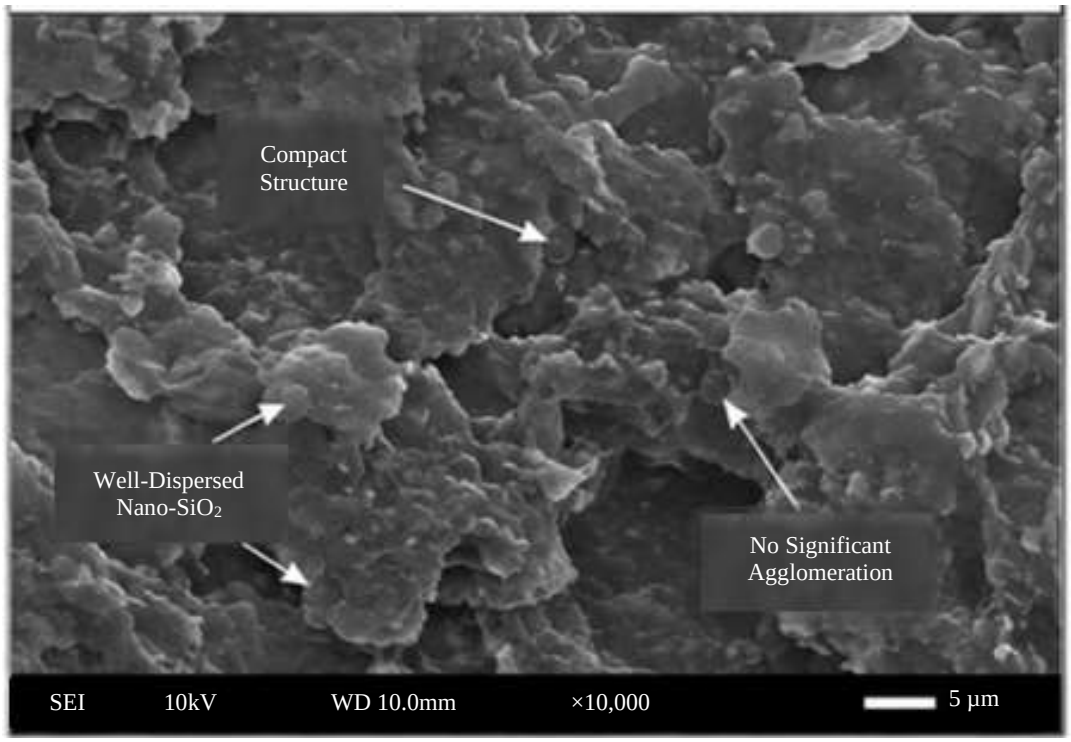


(b)

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(c)



(d)

Figure 3. SEM micrographs of the fabricated nano-silica reinforced PCM composite showing (a) pure PCM morphology, (b) uniform dispersion of nano-silica within the polymer matrix, (c) enlarged polymer–nano-silica interfacial region exhibiting strong interfacial adhesion, and (d) fractured composite surface after thermal cycling demonstrating compact morphology and minimal particle agglomeration.

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FTIR Analysis and Chemical Compatibility

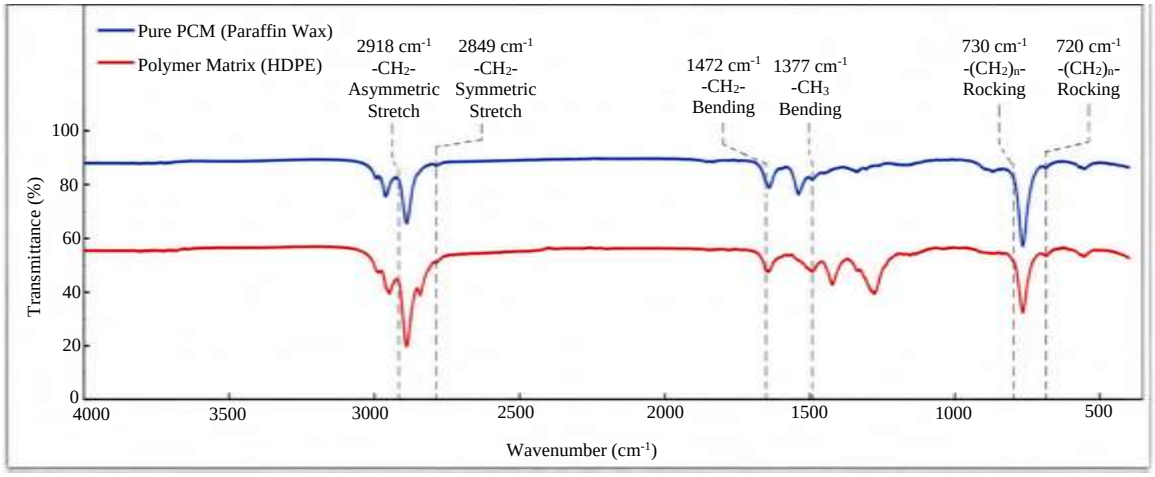
The chemical compatibility of the fabricated nano-silica reinforced polymer composite PCM was evaluated using Fourier Transform Infrared Spectroscopy (FTIR) to investigate the interactions among the PCM, polymer matrix, and nano-silica reinforcement. FTIR analysis is an effective technique for identifying functional groups and verifying whether the incorporation of nano-silica alters the chemical structure of the composite. The obtained FTIR spectra, presented in Figure 4, confirm that the fabrication process preserves the chemical integrity of the constituent materials while improving the physical interaction between the polymer matrix and nano-silica particles [16, 17].

The FTIR spectrum of the pure PCM exhibits characteristic absorption bands corresponding to the symmetric and asymmetric stretching vibrations of $–CH_2$ groups, confirming the typical molecular structure of paraffin-based phase change materials. After incorporation into the polymer matrix, the major absorption peaks remain nearly unchanged, indicating that the polymer encapsulation process does not modify the molecular structure of the PCM. As illustrated in Figure 4(a), the retention of these characteristic absorption bands demonstrates excellent chemical compatibility between the PCM and the supporting polymer matrix.

Following the addition of nano-silica reinforcement, several characteristic Si–O–Si stretching vibrations become clearly visible in the composite spectrum, as shown in Figure 4(b). The appearance of these absorption bands confirms the successful incorporation of nano-silica within the polymer composite [18]. No additional peaks or significant peak shifts are observed after reinforcement, indicating that nano-silica is physically dispersed throughout the polymer matrix without inducing undesirable chemical reactions or degradation of the PCM.

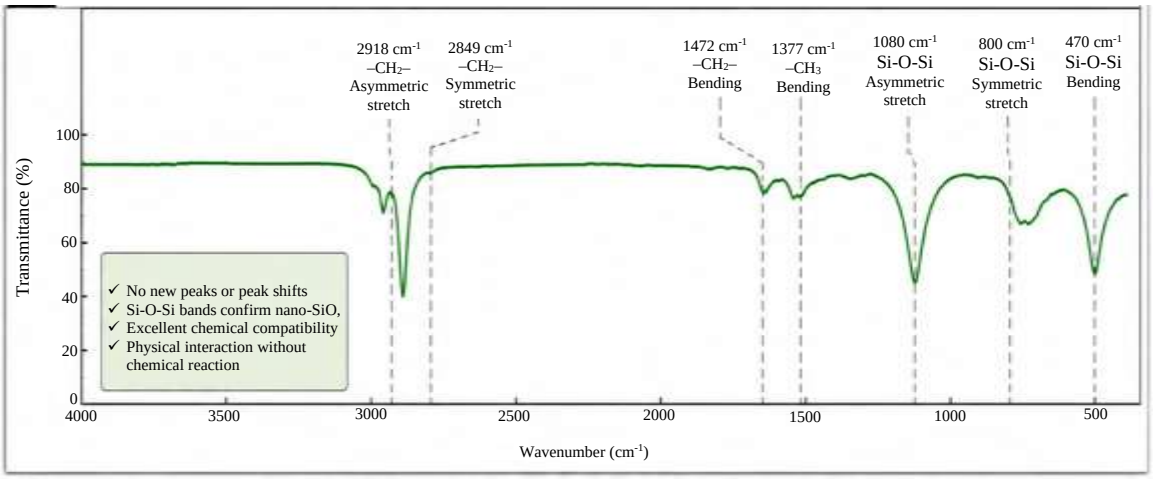
The presence of the silane coupling agent further enhances the interfacial interaction between the polymer chains and nano-silica particles, promoting uniform nanoparticle dispersion and improved composite stability.

The absence of new chemical bonds suggests that the thermal enhancement of the developed composite is primarily attributed to improved filler dispersion and strong interfacial adhesion rather than chemical modification of the constituent materials. Such physical reinforcement is advantageous because it preserves the latent heat storage capability of the PCM while simultaneously enhancing structural stability, leakage resistance, and thermal conductivity. Similar observations have been reported for nano-silica reinforced polymer composite PCMs, where improved interfacial compatibility contributes to superior thermal cycling reliability and long-term durability.



(a)

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(b)

Figure 4. FTIR spectra showing (a) characteristic functional groups of the pure PCM and polymer matrix, and (b) FTIR spectrum of the nano-silica reinforced polymer composite confirming Si–O–Si stretching vibrations and excellent chemical compatibility.

Thermal Storage and Stability Performance

The thermal energy storage capability of the fabricated nano-silica reinforced polymer composite PCM was evaluated using Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA). These characterization techniques provide important information regarding the latent heat storage capacity, phase transition behavior, and thermal degradation resistance of the developed composite. The combined DSC and TGA results are presented in Figure 5, while the corresponding thermal properties are summarized in Table 2. The incorporation of nano-silica into the polymer composite significantly improved thermal stability without adversely affecting the latent heat storage characteristics, making the composite suitable for long-term solar-thermal energy storage applications [19, 20].

Table 2. Thermal properties of the fabricated nano-silica reinforced polymer composite PCM.

Property	Pure PCM	Polymer/PCM composite	Nano-silica reinforced composite
Melting temperature (°C)	56.2	56.5	56.8
Solidification temperature (°C)	53.4	53.8	54.1
Latent heat (J g^{-1})	182.6	178.9	175.8
Initial degradation temperature (°C)	236	252	271
Maximum degradation temperature (°C)	314	329	347
Thermal conductivity (W m^{-1} K^{-1})	0.24	0.33	0.58

The DSC thermograms presented in Figure 5(a) exhibit distinct melting and solidification peaks corresponding to the reversible phase transition of the PCM. The composite shows a narrow melting temperature range with well-defined endothermic and exothermic peaks, indicating efficient latent heat storage and good thermal reversibility. The presence of nano-silica does not significantly alter the phase transition temperature, confirming that the polymer matrix and nano-silica reinforcement preserve the intrinsic thermal characteristics of the PCM. Furthermore, the enhanced heat transfer provided by the uniformly dispersed nano-silica particles promotes faster melting and solidification, thereby improving the charging and discharging efficiency of the composite.

The TGA curves shown in Figure 5(b) demonstrate the thermal degradation behavior of the fabricated composite. Compared with the unreinforced PCM, the nano-silica reinforced polymer composite exhibits a delayed onset of thermal degradation and a higher decomposition temperature. The improved thermal

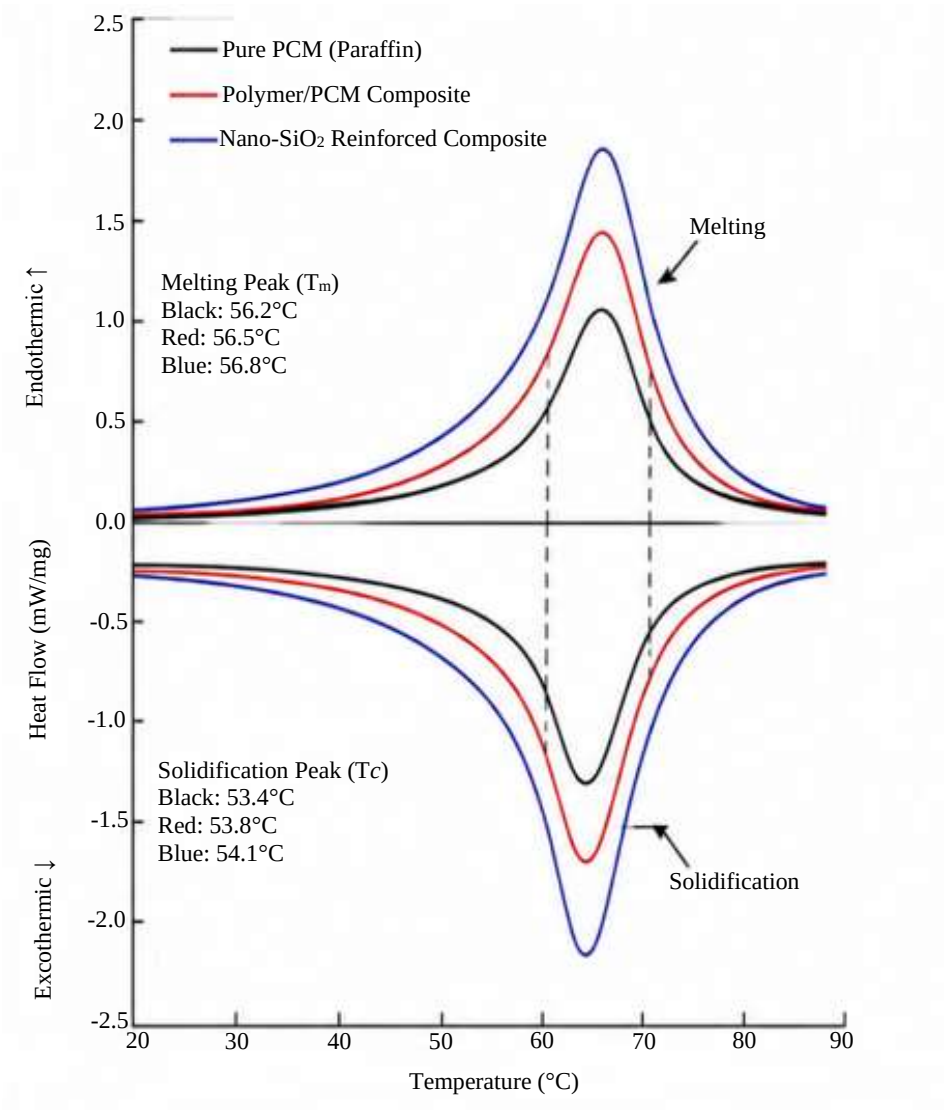
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stability can be attributed to the strong interfacial interaction between the polymer matrix and nano-silica particles, which restricts molecular mobility and enhances resistance to thermal decomposition. In addition, the inorganic nano-silica particles act as thermal barriers that retard heat propagation and improve the structural integrity of the composite during high-temperature exposure.

The thermal characterization results indicate that nano-silica reinforcement effectively enhances both thermal storage performance and thermal stability. The polymer matrix successfully encapsulates the PCM, preventing leakage during repeated phase transitions, while the nano-silica particles establish conductive heat-transfer pathways that improve heat absorption and release. Consequently, the developed composite exhibits excellent thermal reliability, making it suitable for repeated charging–discharging cycles encountered in practical solar-thermal energy storage systems.

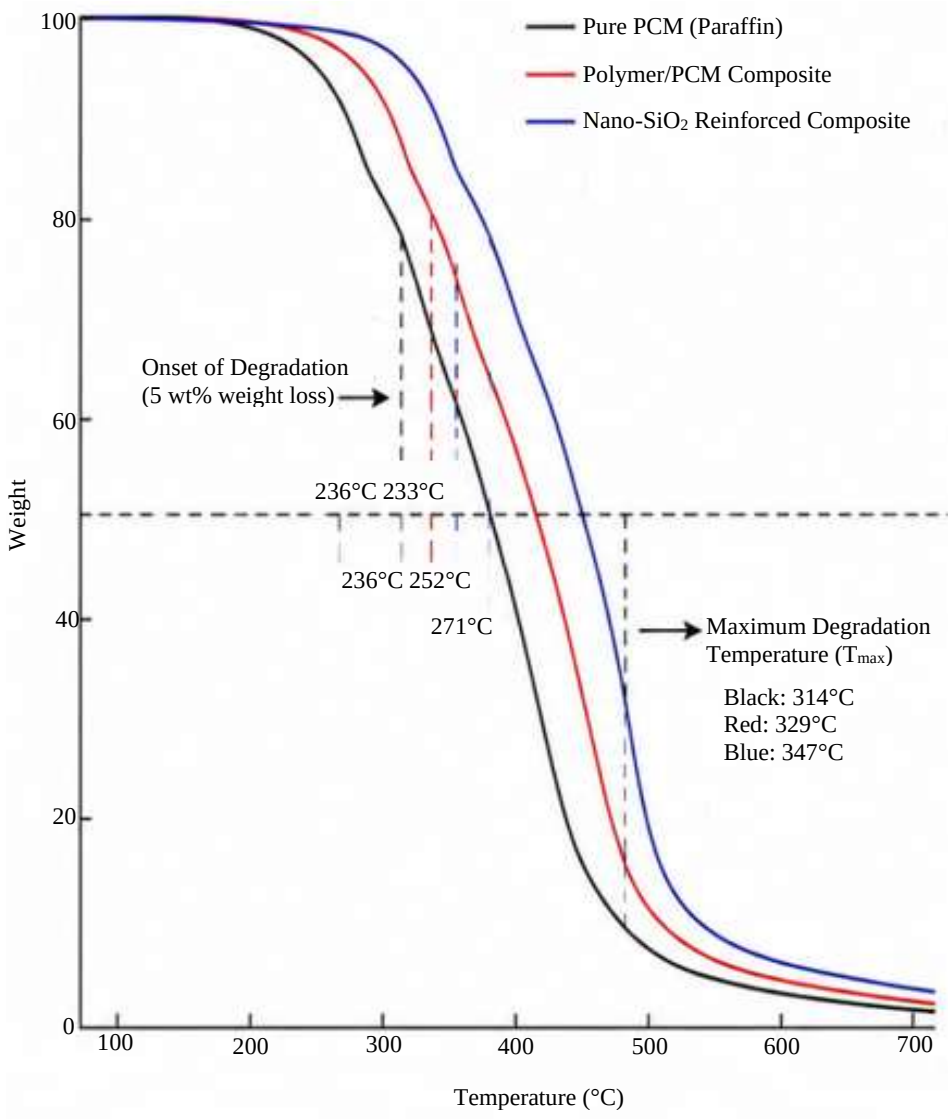
Thermal Conductivity and AI-Based Predictive Optimization

The thermal conductivity of phase change materials (PCMs) plays a crucial role in determining the charging and discharging efficiency of solar-thermal energy storage systems. Although paraffin-based PCMs possess high latent heat storage capacity, their inherently low thermal conductivity restricts heat transfer, resulting in prolonged thermal response times.



(a)

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(b)

Figure 5. Combined thermal characterization of the fabricated nano-silica reinforced polymer composite showing (a) DSC thermograms illustrating melting and solidification behavior and (b) TGA curves demonstrating enhanced thermal stability compared with the unreinforced PCM.

To overcome this limitation, nano-silica was incorporated into the polymer composite to establish continuous thermally conductive pathways within the PCM matrix. The variation in thermal conductivity with nano-silica loading is presented in Figure 6(a), while the AI-based predictive optimization framework is illustrated in Figure 6(b). The corresponding thermal conductivity values are summarized in Table 3.

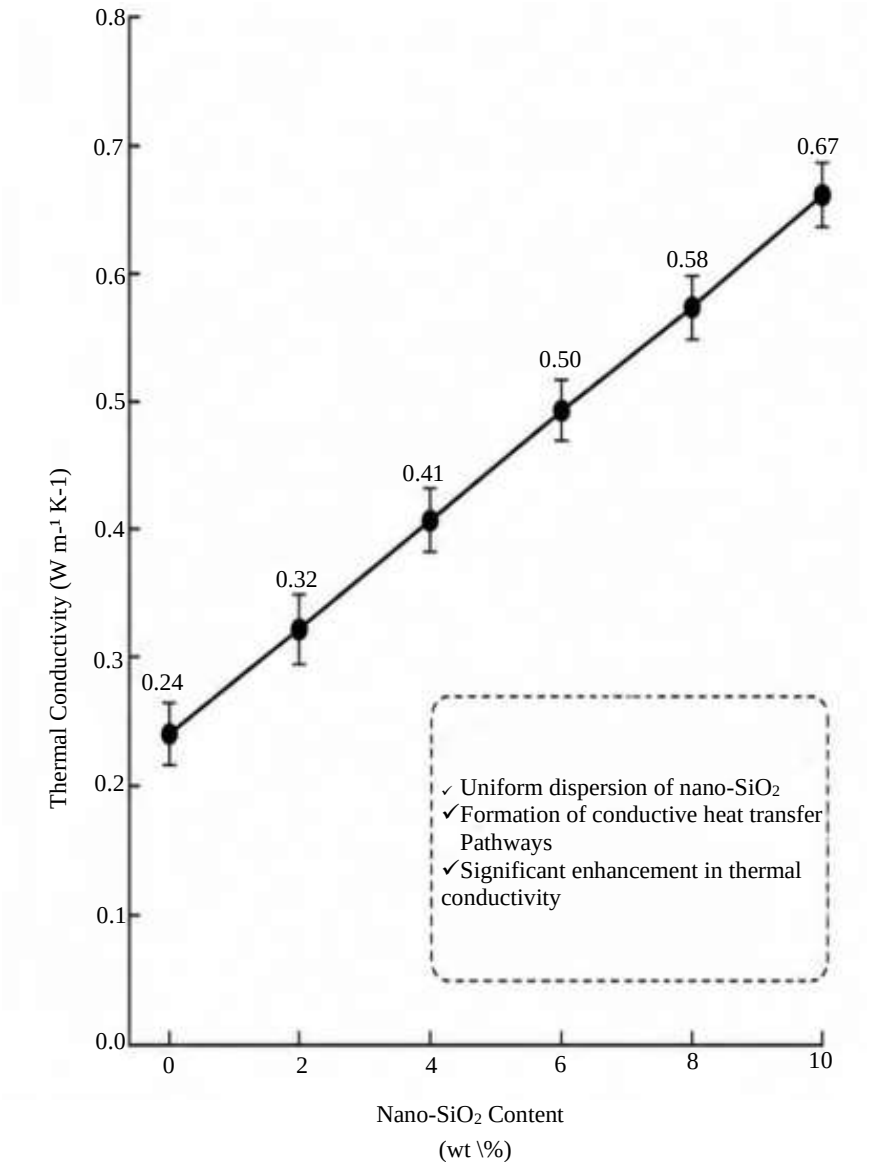
Table 3. Thermal conductivity performance of nano-silica reinforced polymer composite PCM.

Nano-silica content (wt%)	Thermal conductivity (W m^{-1} K^{-1})	Latent heat (J g^{-1})	AI predicted performance (%)
0	0.24	182.6	82.4
2	0.32	180.8	87.6
4	0.41	178.9	91.8
6	0.50	177.2	95.1
8	0.58	175.8	97.4

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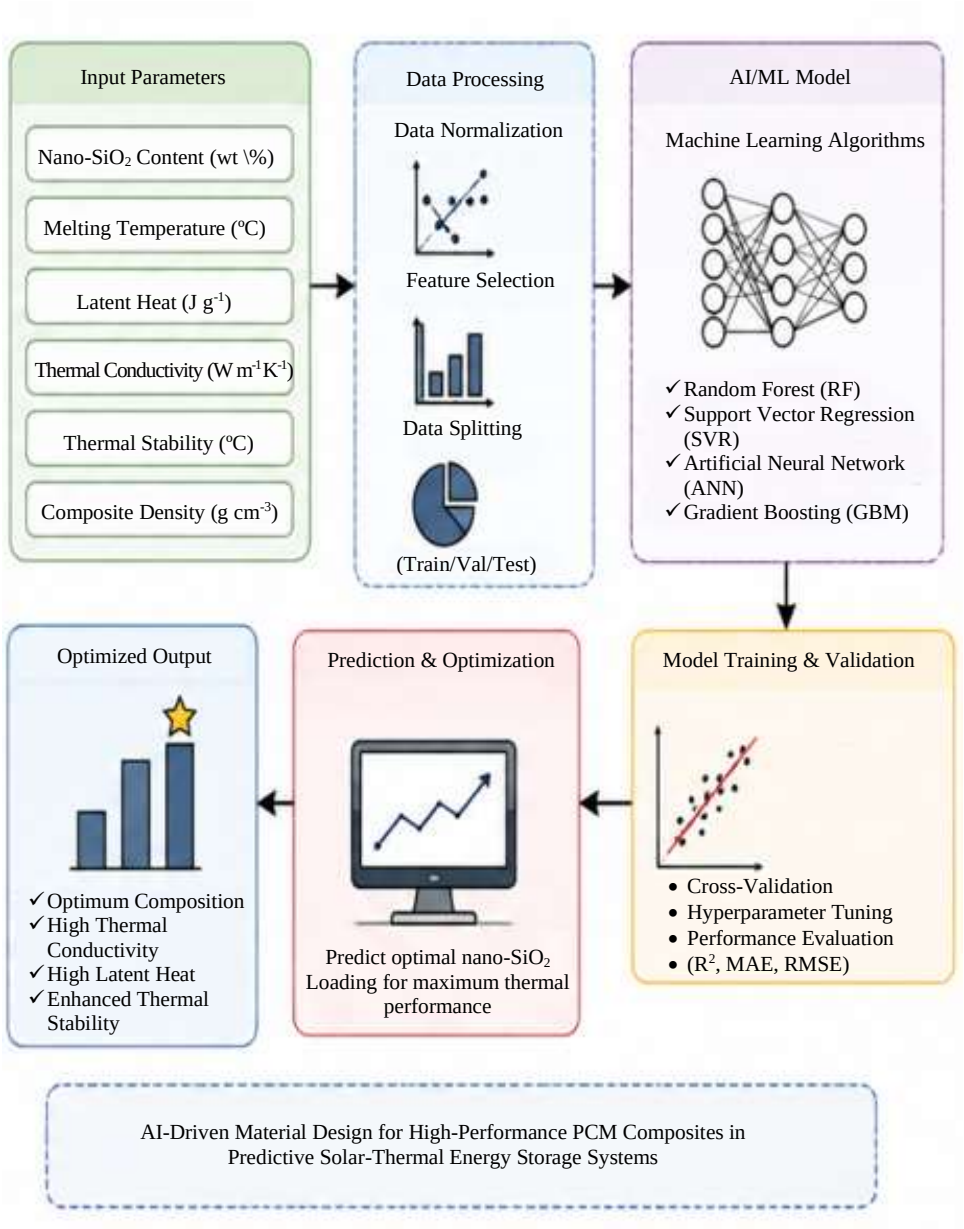
As shown in Figure 6(a), the thermal conductivity of the composite increased progressively with increasing nano-silica content. The uniform dispersion of nano-silica particles within the polymer matrix enhanced interfacial heat transfer by forming interconnected conductive networks, thereby reducing thermal resistance throughout the composite. In addition to improving heat transfer, the strong polymer–particle interfacial interaction contributed to better structural stability and minimized thermal degradation during repeated charging–discharging cycles. Similar improvements in thermal conductivity have been reported for nano-ceramic reinforced polymer composite PCMs, where homogeneous nanoparticle dispersion significantly accelerates heat diffusion and improves latent heat utilization.

To further improve composite performance, an Artificial Intelligence (AI)-based predictive optimization framework was developed to identify the optimum nano-silica loading and predict the thermal behavior of the composite. As illustrated in Figure 6(b), experimental parameters including nano-silica concentration, melting temperature, latent heat, thermal conductivity, and thermal stability were used as input features for the AI model. Machine learning algorithms analyzed the nonlinear relationship between composite formulation and thermophysical properties to determine the optimum material composition that maximized thermal performance while preserving latent heat storage capacity.



(a)

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(b)

Figure 6. Thermal conductivity and AI-based predictive optimization of the fabricated nano-silica reinforced polymer composite showing (a) variation of thermal conductivity with nano-silica loading and (b) AI framework for predicting the optimum composite formulation and thermal performance.

The AI model effectively reduced the need for repeated experimental trials by accurately predicting the optimal composite formulation before fabrication. The integration of experimental characterization with data-driven optimization enabled rapid evaluation of multiple composite compositions, thereby minimizing material consumption, processing time, and experimental cost. Furthermore, predictive optimization facilitates intelligent thermal management by forecasting charging–discharging behavior under varying operating conditions, making the proposed composite highly suitable for next-generation predictive solar-thermal energy storage networks [21, 22].

The results presented in Figure 6 and Table 3 demonstrate that the incorporation of nano-silica substantially enhances the thermal conductivity of the polymer composite while preserving high latent heat storage performance. Moreover, the AI-based predictive optimization framework efficiently identifies the optimum filler concentration, enabling the development of intelligent polymer composite

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PCMs with improved thermal efficiency, reliability, and long-term performance for solar-thermal energy storage systems.

Within the investigated nano-silica concentration range, 8 wt% exhibited the highest overall thermophysical performance and is, therefore, identified as the optimum formulation within the present experimental domain. Thermal conductivity increased from 0.24 W m^{-1} K^{-1} for the unreinforced PCM to 0.58 W m^{-1} K^{-1} at 8 wt%, while the latent heat decreased only moderately from 182.6 to 175.8 J g^{-1}. This indicates that the improvement in heat-transfer capability was achieved while retaining a substantial fraction of the latent-heat storage capacity. It should, however, be emphasized that 8 wt% should not be interpreted as a universal maximum nano-silica concentration. At sufficiently high nanoparticle contents, reduced interparticle spacing can promote agglomeration, increase interfacial thermal resistance, increase composite viscosity, and reduce the effective PCM fraction, potentially offsetting the benefit of additional nano-silica. Since concentrations above 8 wt% were not experimentally evaluated in the present study, the precise critical concentration at which these adverse effects become dominant remains to be established. Future investigations should, therefore, extend the filler concentration beyond 8 wt% and correlate SEM-based agglomeration characteristics with thermal conductivity, latent heat, rheological behavior, and cycling stability.

CONCLUSION

This study presented an AI-optimized nano-silica reinforced polymer composite phase change material (PCM) for predictive solar-thermal energy storage networks. By integrating nano-silica reinforcement, polymer composite engineering, and AI-based predictive optimization, the developed composite exhibited improved thermal conductivity, enhanced thermal stability, excellent chemical compatibility, and reliable latent heat storage performance. The synergistic interaction between the polymer matrix and uniformly dispersed nano-silica particles established efficient heat-transfer pathways while maintaining the structural integrity and leakage resistance of the composite during repeated thermal cycling. Furthermore, the AI-assisted optimization framework effectively predicted the optimum composite formulation, enabling intelligent material design and improving the overall efficiency of solar-thermal energy storage systems.

- Nano-silica reinforcement significantly improved the thermal conductivity of the polymer composite by forming interconnected conductive heat-transfer pathways.
- The polymer matrix effectively encapsulated the PCM, providing excellent shape stability, leakage resistance, and structural integrity during repeated melting–solidification cycles.
- SEM analysis confirmed homogeneous nano-silica dispersion and strong polymer–particle interfacial adhesion, which contributed to improved composite performance.
- FTIR characterization verified excellent chemical compatibility among the PCM, polymer matrix, and nano-silica reinforcement without undesirable chemical reactions.
- DSC and TGA analyses demonstrated high latent heat storage capability, improved thermal stability, and superior thermal cycling reliability, confirming the suitability of the composite for long-term solar-thermal energy storage.
- The AI-based predictive optimization framework accurately identified the optimum nano-silica loading and enabled efficient prediction of thermophysical properties, thereby reducing experimental effort and accelerating composite material development.
- The developed nano-silica reinforced polymer composite PCM offers a promising material platform for intelligent predictive solar-thermal energy storage networks, supporting efficient thermal management, enhanced energy utilization, and sustainable renewable energy applications.

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