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Research Paper

Numerical Investigation of ZnS Particle Size Effects on Optical Performance and Color Quality of Phosphor-Converted White LEDs

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Abstract
This study presents a numerical investigation of the influence of ZnS particle size on the optical performance and color quality of phosphor-converted white light-emitting diodes (pc-WLEDs) using Mie-scattering theory combined with Monte Carlo optical simulations. The effects of ZnS particle size on light-scattering behavior, luminous flux, color rendering index (CRI), and color quality scale (CQS) have not been systematically evaluated. The simulation results indicate that increasing the ZnS particle size enhances light scattering but simultaneously reduces luminous flux and degrades color uniformity and color-rendering performance. In contrast, smaller ZnS particles exhibit lower scattering coefficients while maintaining higher luminous output, CRI, and CQS values. These findings demonstrate the trade-off between scattering enhancement and optical performance and highlight the importance of optimizing ZnS particle size to achieve an appropriate balance between luminous efficiency and color quality in pc-WLEDs. The results provide useful design guidelines for the development of high-performance phosphor-converted pc-WLEDs. Future work should focus on experimental validation and the investigation of hybrid scattering-particle systems for further performance enhancement.

Keywords
pc-WLEDs, ZnS Nanoparticles, Mie-Scattering Theory, Optical Scattering

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1. INTRODUCTION

The demand for high-performance and energy-efficient lighting solutions has driven significant advancements in light-emitting diode (LED) technology. As a cornerstone of modern lighting, LEDs have revolutionized a wide range of applications, from residential and commercial illumination to automotive and display technologies. Despite their widespread adoption, LEDs still encounter several critical challenges that limit their performance and broader applicability, including inefficient light extraction processes, non-uniform angular color distribution, and poor stability in color rendering and correlated color temperature (CCT) (Anh and Lee, 2024; Le et al., 2022; Tung et al., 2024a).

To overcome these challenges, researchers and engineers have explored various materials and techniques. One of the most extensively investigated approaches is phosphor optimization (Kumari et al., 2025; Zhang et al., 2023; Tung et al., 2024b). Efforts have been made to develop high-efficiency phosphors (e.g., YAG:Ce^{3+}) and hybrid phosphor systems that offer better color quality and thermal stability (Khan et al., 2024; Thuy et al., 2022). Phosphor geometry and placement in LED packaging have also been optimized to improve angular uniformity (Le et al., 2022; Trang et al., 2025). However, phosphor combinations aimed at achieving optimal white-light performance often require complex fabrication techniques and processing procedures, increasing production costs (Loan and Anh, 2021; Thi et al., 2020). Another feasible solution for overcoming these issues is to reduce total internal reflection and enhance scattering efficiency within LED packages (Ma et al., 2024; Loan et al., 2025; Gelbing et al., 2026). Reported strategies include incorporating scattering particles into phosphor layers, modifying LED structures (e.g., LED chip surface texturing, nanopatterning, and microlens arrays), and applying advanced coatings with high refractive indices, anti-reflective properties, or enhanced thermal stability (Li et al., 2026; Chen et al., 2020). Such approaches have been shown to reduce internally trapped light by enhancing scattering efficiency, particularly through the use of materials with high refractive indices (Le et al., 2021; That et al., 2020). Particularly, in LED lighting systems, scattering materials play a dual role: they enhance light extraction by reducing total internal reflection and improve color mixing by diffusing light across the visible spectrum (Anh and Ngoc, 2020). Various scattering materials, including $BaSO_4$, ZrO_2, TiO_2, and SiO_2, have been incorporated into LED packaging to enhance light extraction and diffusion. $BaSO_4$ provides excellent diffuse reflectivity but has limited thermal stability (Anh et al., 2025). ZrO_2 offers strong scattering and high thermal stability but is costly. TiO_2 provides the strongest scattering but can distort color (Chakrabarti and Alessandri, 2024). SiO_2 enhances uniformity but exhibits relatively low scattering efficiency (Cong and Anh, 2025; Loan et al., 2022). Therefore, investigating alternative scattering materials could provide manufacturers with greater flexibility in meeting specific LED performance requirements. Among various materials, zinc sulfide (ZnS) has emerged as a promising solution to many of these challenges. With its high refractive index (~2.35), wide bandgap (~3.6 eV), and excellent scattering properties, ZnS enables superior light extraction and uniformity in pc-WLEDs. Unlike conventional scattering materials, ZnS offers a unique combination of strong light scattering, a high refractive index, and tunable optical properties (Loan et al., 2026). These characteristics make ZnS particularly well-suited for addressing issues such as angular color uniformity, correlated color temperature consistency, and luminous efficacy. Additionally, ZnS exhibits good thermal stability and is environmentally friendly, making it a sustainable choice for advanced LED applications. This paper investigates the potential of ZnS as a scattering material in LEDs, focusing on its impact on key performance parameters such as scattering coefficient, CCT, CRI, CQS, and luminous efficacy. The Mie-scattering theory and Monte Carlo simulations implemented in MATLAB are employed to model the effects of ZnS particle size on light scattering behaviors. The simulation results indicate that ZnS has the potential to serve as an effective alternative to conventional scattering materials and offers a promising strategy for enhancing the optical performance of pc-WLEDs.

Although various scattering particles such as TiO_2, SiO_2, $BaSO_4$, and ZnO have been extensively investigated to improve the optical performance of phosphor-converted white light-emitting diodes (pc-WLEDs), relatively little attention has been devoted to the use of ZnS nanoparticles as scattering enhancement materials. Owing to its relatively high refractive index, high optical transparency across the visible spectrum, and excellent thermal stability, ZnS offers a promising alternative for achieving an optimal balance between luminous efficiency and color quality in LED packaging systems. In addition, most previous studies have focused either on enhancing luminous flux or improving color uniformity individually, while the combined influence of ZnS particle size on scattering behavior, luminous performance, correlated color temperature (CCT) stability, color rendering index (CRI), and color quality scale (CQS) has not been systematically evaluated.

Therefore, this study aims to numerically evaluate the influence of ZnS particle size on the optical characteristics of pc-WLEDs using Mie-scattering theory and Monte Carlo optical simulations. The results provide insights into the trade-off between scattering enhancement and color quality preservation, thereby providing practical guidelines for the design and development of future LED packaging systems.

2. EXPERIMENTAL SECTION

A phosphor-converted white LED (pc-WLED) package consisting of a blue LED chip, a YAG:Ce^{3+} phosphor layer, and uniformly dispersed ZnS scattering particles was considered in this study. The ZnS particles were incorporated into the phosphor layer to investigate their influence on light scattering behavior and optical performance. The particle radii of 13, 15, and 17 nm were selected to evaluate the effect of nanoscale size variation on the optical characteristics of the LED package. The optical scattering behavior of ZnS nanoparticles embedded in the phosphor layer was investigated using the classical Mie-scattering theory. This theoretical approach is widely employed to describe the interaction between electromagnetic radiation and spherical particles whose dimensions are comparable to the wavelength of the incident light. In the present study, ZnS particles were assumed to be homogeneous and spherical, allowing their scattering characteristics to be accurately evaluated through the Mie formalism. The scattering coefficient, scattering cross-section, and angular scattering distribution were calculated according to Equations (1)–(8). These equations relate the optical response of ZnS particles to their radius, refractive index, and the wavelength of incident light. The calculations were performed over the visible spectral range of 380–780 nm, which corresponds to the operating spectrum of phosphor-converted white LEDs.

Since the scattering efficiency is strongly dependent on the size parameter $x = 2\pi r/\lambda$, variations in ZnS particle radius can significantly alter the propagation and redistribution of light within the phosphor layer. Consequently, the Mie-scattering model provides an effective framework for evaluating the influence of ZnS particle size on the optical performance, color quality, and luminous characteristics of pc-WLEDs systems.

$$\mu_{sca}(\lambda) = \int N(r) C_{sca}(\lambda, r) dr \tag{1}$$

where $N(r)$ represents the number density of scattering particles (mm^{-3}), C_{sca} denotes the scattering cross-section (mm^2), λ represents the incident light wavelength (nm), and r indicates the radius of particles (μm) respectively. The following expression is used to calculate C_{sca} based on Mie theory:

$$C_{sca} = \frac{2\pi}{k^2} \sum_{1}^{\infty} (2n-1)(|a_n|^2 + |b_n|^2) \tag{2}$$

where $k = 2\pi/\lambda$, and a_n and b_n are calculated as follows:

$$a_n(x, m) = \frac{\psi_n'(mx)\psi_n(x) - m\psi_n(mx)\psi_n'(x)}{\psi_n'(mx)\xi_n(x) - m\psi_n(mx)\xi_n'(x)} \tag{3}$$

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$$b_n(x,m) = \frac{m\psi_n'(mx)\psi_n(x) - \psi_n(mx)\psi_n'(x)}{m\psi_n'(mx)\xi_n(x) - \psi_n(mx)\xi_n'(x)} \quad (4)$$

where $x = kr$, m is the refractive index, and $\psi_n(x)$ and $\xi_n(x)$ are the Riccati–Bessel functions. The coefficients a_n and b_n describe the scattering response of spherical particles and are functions of both the particle size parameter and the refractive-index contrast between the particle and the surrounding medium.

The phase function is expressed as follows:

$$p(\theta,\lambda,r) = \frac{4\pi\beta(\theta,\lambda,r)}{k^2 C_{sca}(\lambda,r)} \quad (5)$$

The phase function characterizes the angular redistribution of scattered light and plays an important role in determining the optical transport behavior within the phosphor layer. Here, $\beta(\theta,\lambda,r)$, $S_1(\theta)$ and $S_2(\theta)$ represent the angular scattering amplitudes, which are computed as follows:

$$\beta(\theta,\lambda,r) = \frac{1}{2}\left[|S_1(\theta)|^2 + |S_2(\theta)|^2\right] \quad (6)$$

$$S_1 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)}\left[a_n(x,m)\pi_n(\cos\theta) + b_n(x,m)\tau_n(\cos\theta)\right] \quad (7)$$

$$S_2 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)}\left[a_n(x,m)\tau_n(\cos\theta) + b_n(x,m)\pi_n(\cos\theta)\right] \quad (8)$$

The Mie formalism enables accurate prediction of scattering behavior over the visible spectral range. Since the size parameter $x = 2\pi r/\lambda$ directly depends on the ZnS particle radius, increasing the ZnS particle size is expected to modify both scattering intensity and angular distribution, thereby affecting the luminous output and color quality metrics of the simulated pc-WLEDs package.

Table 1. Simulation Parameters

Parameter	Value
ZnS particle radius	13, 15, 17 nm
Wavelength range	380–780 nm
Simulation platform	MATLAB
Particle shape	Spherical
Distribution	Monodisperse
Phosphor	$YAG:Ce^{3+}$

All simulations (Table 1) were performed under identical optical conditions to isolate the influence of ZnS particle size. Monodisperse particle distributions were assumed to simplify the analysis and facilitate a direct comparison among different particle radii. The optical properties were calculated in MATLAB using the Mie-scattering equations described above. The scattering coefficient was first determined as a function of wavelength and ZnS particle radius. The resulting scattering characteristics were then used to evaluate their influence on luminous flux, correlated color temperature (CCT), D-CCT, color rendering index (CRI), and color quality scale (CQS). Finally, the optical performance associated with different ZnS particle sizes was compared and analyzed.

Table 2. Optical Quantities Calculated in This Study

Quantity	Description
μ_{sca}	Scattering coefficient
Luminous flux	LED optical output
CCT	Correlated color temperature
D-CCT	CCT deviation
CRI	Color rendering index
CQS	Color quality scale

The optical quantities listed in Table 2 were selected to comprehensively evaluate the influence of ZnS particle size on the performance of phosphor-converted white LEDs. The scattering coefficient (μ_{sca}) was employed to characterize the scattering capability of ZnS nanoparticles, while luminous flux was used to assess the optical output of the LED package. Correlated color temperature (CCT) and D-CCT were analyzed to evaluate color stability and angular color uniformity. In addition, the color rendering index (CRI) and color quality scale (CQS) were calculated to investigate the effects of scattering behavior on color reproduction and overall lighting quality. These parameters collectively provide a comprehensive assessment of the trade-off between scattering enhancement and optical performance in ZnS-based pc-WLEDs systems.

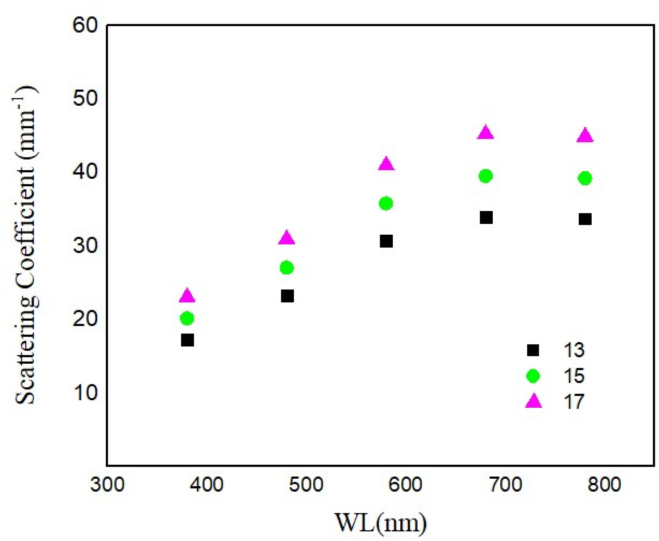

Figure 1. Scattering Coefficient as a Function of Wavelength for Different ZnS Particle Radius

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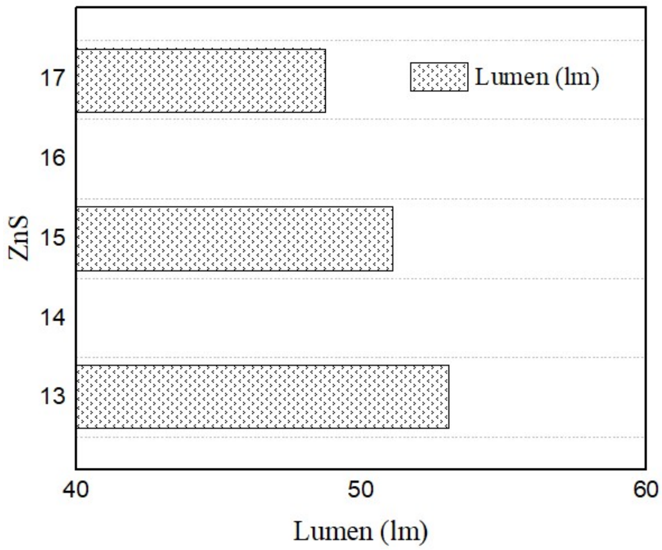

Figure 2. Luminous Flux as a Function of ZnS Particle Radius

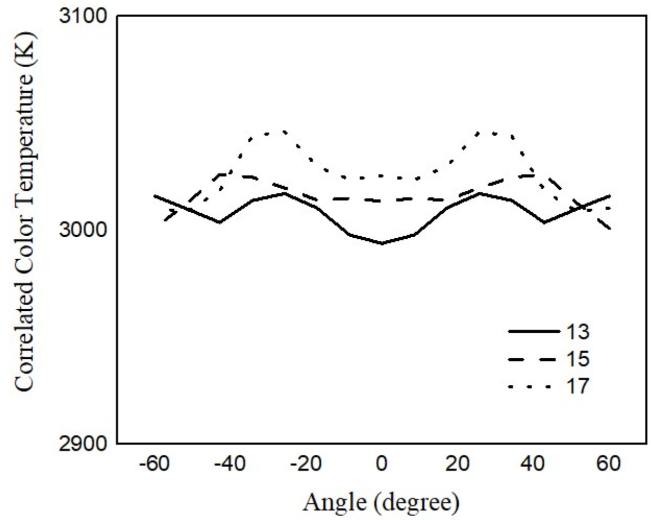

Figure 3. Angular Variation of Correlated Color Temperature for Different ZnS Particle Radius

3. RESULTS AND DISCUSSION

Figure 1 illustrates the scattering coefficient as a function of wavelength (WL) for different ZnS particle radii (13, 15, and 17 nm). The scattering coefficient increases significantly with particle size and wavelength, especially for larger particles. This trend indicates that larger ZnS particles enhance scattering in the LED light field, particularly at longer wavelengths (e.g., the red region), which may improve light extraction and color uniformity. The size-dependent scattering efficiency is consistent with Mie-scattering theory, which predicts that particle size directly impacts the interaction of light with the material. This suggests that selecting appropriate ZnS particle sizes may help optimize the optical performance of white LEDs.

Figure 2 illustrates the luminous flux (lm) of LEDs as a function of ZnS particle radius. The results show a clear trend: larger ZnS particles (17 nm) produce lower luminous flux than smaller particles (13 nm). The reduction in luminous flux can be primarily attributed to increased scattering-induced optical losses. As the particle size increases, photons experience more scattering events within the phosphor layer, leading to longer optical paths and a higher probability of light trapping. Consequently, less optical energy contributes to useful light extraction, resulting in a decrease in luminous flux.

Figure 3 shows how the correlated color temperature (CCT) changes with the angle of observation for different ZnS particle radii. The fluctuation of CCT across different observation angles indicates that smaller ZnS particles (13 nm) provide better angular color uniformity compared to larger particles. This angular dependency is critical for LED applications requiring consistent color rendering, such as in display backlighting or architectural lighting. Larger particles (17 nm), while providing higher scattering coefficients, appear to compromise angular uniformity, potentially leading to undesirable visual artifacts. Figure 4 examines the deviation of correlated color temperature (D-CCT), which measures the difference in CCT across the angular range, as a function of ZnS particle size. D-CCT increases with particle size, indicating that larger ZnS particles create greater CCT variations. Excessive scattering from larger particles may lead to internal light losses or angular non-uniformity, which must be addressed to ensure efficient and high-quality lighting. This finding suggests that selecting appropriate particle sizes for different applications is important for achieving the desired light quality and color consistency. For general lighting applications, minimizing D-CCT is essential to ensure uniform illumination. Figure 5 examines the impact of ZnS particle size on the color

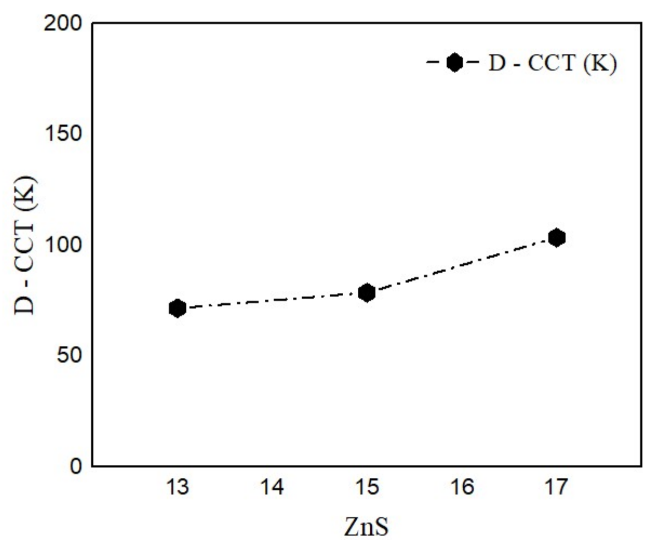

Figure 4. Variation in D-CCT as a Function of ZnS Particle Radius

rendering index (CRI), a measure of the LED's ability to accurately reproduce colors. The CRI values decrease slightly as the ZnS particle size increases, with the highest CRI observed for smaller particles (13 nm). The decrease in CRI with increasing ZnS particle size may be associated with changes in the spatial redistribution of light caused by stronger scattering. Excessive scattering can influence the balance of optical energy within the phosphor layer and reduce the effectiveness of color mixing, leading to slightly lower CRI values. Figure 6 presents the color quality scale (CQS), which evaluates both color rendering and visual preference, as a function of ZnS particle size. Similar to the CRI trend, the CQS values decrease with increasing particle size. The highest CQS value is achieved with the smallest ZnS particles (13 nm), indicating that they provide superior overall color quality. The reduction in CQS observed for larger ZnS particles indicates that excessive scattering may negatively influence overall lighting quality. Although stronger scattering improves light diffusion, it may also reduce the effectiveness of color mixing and angular color consistency, resulting in lower CQS values.

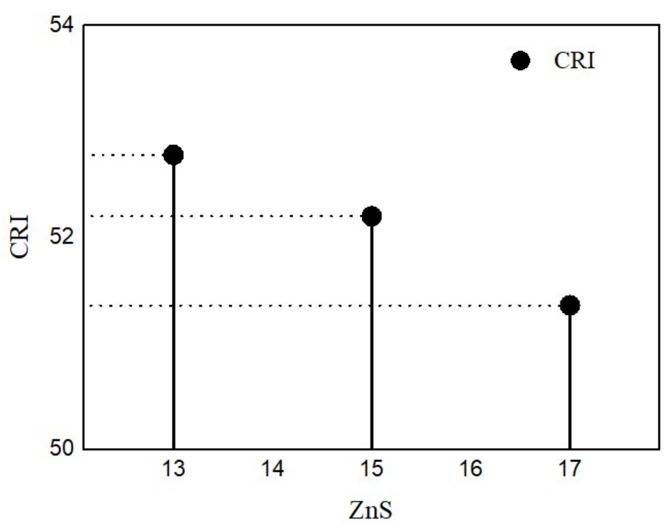

Figure 5. CRI as a Function of ZnS Particle Radius

To verify the reliability of the simulation results, the observed trends were compared with those reported in previous studies employing scattering particles in phosphor-converted LEDs. Similar to TiO_2, $BaSO_4$, and ZnO scattering materials, larger particle sizes generally lead to increased scattering coefficients due to the stronger interaction between incident photons and particles. However, excessive scattering may also increase optical path lengths and reduce angular color uniformity. The present simulation results indicate that increasing ZnS particle size enhances scattering efficiency but simultaneously reduces luminous flux, CRI, and CQS values. This behavior is consistent with previous reports on TiO_2 and ZnO scattering particles, where stronger scattering improves light diffusion but may negatively influence color quality metrics. Therefore, the observed trends are physically reasonable and consistent with established scattering mechanisms reported in the literature. These comparisons support the validity of the numerical model and demonstrate that ZnS exhibits optical behavior comparable to that of other scattering materials commonly employed in pc-WLEDs (Chen et al., 2020; Trang et al., 2025; Tung et al., 2024b).

Several limitations should be acknowledged in the present study. First, the investigation is based entirely on numerical simulations and does not include experimental fabrication or characterization of ZnS nanoparticles. Second, monodisperse particle distributions were assumed, whereas practical materials often exhibit broader particle size distributions. Third, thermal effects, particle agglomeration, and long-term material degradation were not considered in the simulation model. Future studies should combine experimental characterization techniques, such as XRD, SEM, TEM, and optical spectroscopy, with numerical simulations to further validate the predicted trends and provide a more comprehensive understanding of ZnS scattering behavior in phosphor-converted white LEDs.

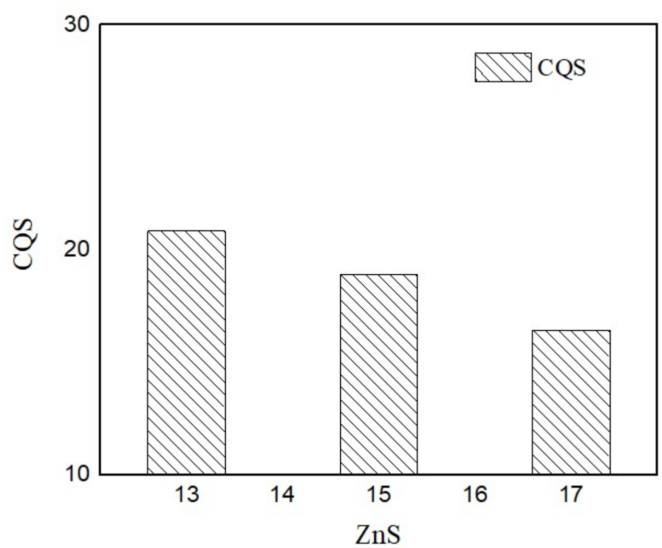

Figure 6. CQS as a Function of ZnS Particle Radius

4. CONCLUSIONS

The simulation results indicate the critical role of ZnS particle size in determining the optical, luminous, and color rendering properties of LEDs. Larger ZnS particles significantly enhance scattering efficiency. However, this comes at the cost of reduced LED optical performance, including luminous flux, CCT uniformity, CRI and CQS, which are better preserved with smaller ZnS particles. These findings emphasize that although scattering enhancement provides significant benefits for the optical performance of LEDs, it must be carefully controlled to avoid undesirable performance degradation caused by excessive scattering-induced optical losses. This underscores the importance of selecting appropriate particle sizes for application-specific LED

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performance. To address this balance, future research could explore hybrid particle systems combining different particle sizes, advanced phosphor compositions to improve spectral uniformity, and tailored scattering layers for enhanced light extraction. By carefully tailoring ZnS particle properties, LED technology can meet the diverse demands of general lighting, display systems, and specialized environments requiring precise color rendering and uniformity. These findings provide preliminary evidence supporting the potential application of ZnS nanoparticles as scattering materials in phosphor-converted white LEDs. Further experimental validation is required to confirm the predicted trends.

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