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Influence of 2-Mercaptopyridine on the Structural and Functional Behavior of Polyphenylene Sulfide

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Abstract - The modification of high-performance polymers through small functional molecules offers an effective route for tuning their structural and functional characteristics. In the present study, the influence of 2-mercaptopyridine on the structural and functional behavior of polyphenylene sulfide is systematically examined to elucidate the underlying molecular interactions and their consequences on material performance. Particular emphasis is placed on understanding how the incorporation of 2-mercaptopyridine affects the polymer framework at the molecular level. Structural analysis reveals that the interaction between polyphenylene sulfide chains and 2-mercaptopyridine induces noticeable changes in molecular organization and electronic distribution. These modifications contribute to altered functional behavior, including variations in electronic response and overall material stability. The study further highlights the role of sulfur- and nitrogen-containing functionalities in facilitating intermolecular interactions, leading to enhanced electronic communication within the polymer system. The observed changes in functional behavior are closely correlated with modifications in molecular structure, demonstrating a clear structure–function relationship. This work provides valuable insights into the controlled modification of polyphenylene sulfide using heteroatom-rich molecules and underscores the importance of molecular-level design strategies for optimizing polymer properties. The findings are expected to support the development of advanced polymer systems with tunable characteristics suitable for emerging applications in functional materials, electronics, and related technologies.

Keywords - Polyphenylene sulfide; 2-mercaptopyridine; Polymer modification; Structural behavior; Functional properties; Structure–function relationship; Advanced polymer materials

1. INTRODUCTION

1.1 High-Performance Polymers and Functional Tailoring

High-performance polymers have emerged as indispensable components in advanced material technologies due to their exceptional thermal stability, mechanical robustness, and chemical resistance. These materials play a critical role in modern electronics, aerospace components, energy storage devices, and functional coatings, where long-term reliability under demanding operational conditions is required [1,2]. Unlike conventional polymers, high-performance systems exhibit rigid backbones and enhanced intermolecular interactions, enabling them to maintain structural integrity at elevated temperatures and under harsh chemical environments.

Among this class of materials, polyphenylene sulfide (PPS) has attracted sustained attention owing to its unique combination of aromatic rigidity and sulfur-containing linkages. The presence of sulfide bridges within the polymer backbone contributes to enhanced thermal endurance, dimensional stability, and resistance to oxidative degradation [3]. Additionally, the aromatic nature of PPS facilitates electron delocalization along the backbone, making it a promising candidate for functional and electronic applications beyond traditional structural uses. However, despite these intrinsic advantages, pristine PPS often exhibits limited tunability of functional properties, necessitating targeted modification strategies to expand its applicability in advanced functional systems.

1.2 Small-Molecule–Induced Property Modulation

In recent years, the modification of polymer systems through the incorporation of small functional molecules has emerged as an effective and versatile approach for tailoring material properties without altering the fundamental polymer backbone [4]. Unlike bulk copolymerization or extensive chemical grafting, small-molecule modification allows fine control over local molecular environments, enabling precise tuning of electronic, optical, and stability-related characteristics. This strategy is particularly attractive for high-performance polymers, where preserving the inherent structural advantages while introducing new functionalities is of paramount importance.

Heteroatom-rich molecules have proven especially effective in this context due to their ability to participate in diverse intermolecular interactions, including charge transfer, dipole–dipole coupling, and soft-atom coordination [5]. Sulfur- and nitrogen-containing functional groups, in particular, are known to influence electron density distribution and intermolecular organization within polymer matrices. When judiciously selected, such molecules can act as molecular modulators that enhance electronic communication and functional responsiveness without compromising the polymer's thermal or mechanical stability. Consequently, understanding the molecular-level interactions between high-performance polymers and heteroatom-rich modifiers has become a key research focus in the development of next-generation functional materials.

1.3 Significance of 2-Mercaptopyridine as a Functional Modifier

2-Mercaptopyridine represents a unique class of functional molecules that combines sulfur and nitrogen heteroatoms within a compact aromatic framework. The coexistence of a thiol group and a pyridine nitrogen endows this molecule with dual interaction capability, allowing it to engage in both soft sulfur-based interactions and directional nitrogen-mediated electronic coupling [6]. Such cooperative functionality makes 2-mercaptopyridine particularly suitable for interacting with sulfur-rich polymer systems such as PPS.

From a molecular interaction perspective, the introduction of 2-mercaptopyridine into a PPS framework is expected to influence local electronic distribution and intermolecular organization through heteroatom–heteroatom proximity effects. The sulfur atoms of PPS can interact synergistically with the thiol and pyridine functionalities, potentially leading to enhanced electronic communication pathways and modified charge distribution along the polymer chains. This dual-heteroatom interaction mechanism distinguishes 2-mercaptopyridine from commonly used single-function modifiers and introduces a level of molecular complexity that has not been extensively explored in PPS-based systems. As a result, the use of 2-mercaptopyridine offers a novel route for probing and controlling structure-driven functional behavior in high-performance polymers.

1.4 Motivation and Scope of the Present Study

Despite extensive studies on PPS for structural and industrial applications, investigations focusing on its controlled functional modification at the molecular level remain relatively limited. Existing literature primarily addresses macroscopic property enhancement through fillers, blends, or copolymerization strategies, often overlooking the subtle yet crucial role of small-molecule–induced electronic and structural modulation [7,8]. Moreover, the specific influence of heteroatom-rich molecules containing cooperative sulfur and nitrogen functionalities on PPS has not been systematically elucidated.

The present study is motivated by the need to bridge this knowledge gap by providing a detailed molecular-level examination of how 2-mercaptopyridine interacts with the PPS framework and alters its structural and functional behavior. By correlating changes in molecular organization and electronic distribution with observed functional responses, this work aims to establish a clear structure–function relationship. The scope of the study extends beyond property observation, focusing instead on fundamental interaction mechanisms that govern functional evolution in modified PPS systems. Such insights are expected to contribute to rational design strategies for high-performance polymers with tunable characteristics, supporting their integration into emerging applications in functional materials, electronics, and advanced technologies.

2. MOLECULAR DESIGN AND INTERACTION FRAMEWORK

2.1 Structural Characteristics of Polyphenylene Sulfide

Polyphenylene sulfide (PPS) is a high-performance engineering polymer that combines an aromatic backbone with sulfur-based linkages, resulting in exceptional thermal, chemical, and mechanical stability. The polymer's rigidity is primarily imparted by the para-linked phenyl units, which constrain rotational flexibility and preserve the structural integrity of the chain under high-temperature and chemically harsh environments. The sulfide bridges contribute not only to chain connectivity but also to electronic polarizability, enabling partial delocalization of π-electrons along the backbone. This electronic delocalization enhances the intrinsic conductivity and electronic responsiveness of PPS, making it suitable for functional and electronic applications in addition to its conventional use in structural components [9].

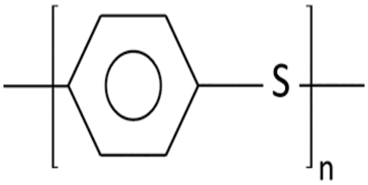

Figure 1:chemical Structure of PPS

The polymer chain packing in PPS is largely dictated by the interplay between aromatic stacking and intermolecular van der Waals interactions. While the polymer exhibits semi-crystalline regions, the local ordering can be sensitive to external perturbations such as the incorporation of small functional molecules. Subtle disruptions in chain packing or conformational adjustments at the local level can significantly influence the polymer's electronic and optical behavior, highlighting the potential for controlled functionalization at the molecular scale.

2.2 Molecular Features of 2-Mercaptopyridine

2-Mercaptopyridine is a heteroaromatic small molecule characterized by the coexistence of a thiol (-SH) group and a pyridine nitrogen atom within a compact aromatic ring. The thiol group acts as a soft donor capable of engaging in non-covalent interactions with sulfur-rich polymer backbones, while the pyridine nitrogen functions as a Lewis base, participating in directional donor–acceptor interactions [9]. The asymmetric electronic distribution arising from this dual-heteroatom arrangement allows 2-mercaptopyridine to influence both the structural and electronic properties of the surrounding polymer matrix.

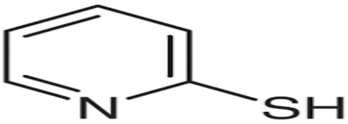

Figure 2:Chemical Structure of 2-Mercaptopyridine

The donor–acceptor nature of 2-mercaptopyridine facilitates partial charge transfer when it interacts with PPS chains, thereby modulating the local electronic environment. Additionally, the aromatic nature of the molecule enables π–π stacking interactions with the phenyl rings of PPS, providing further stabilization and ordering at the microstructural level. These combined features make 2-mercaptopyridine a versatile molecular modulator capable of inducing tunable structural and functional modifications in PPS.

2.3 Hypothesized Interaction Mechanisms

The PPS–2-mercaptopyridine system is expected to be governed by multiple non-covalent interactions. The sulfur atoms in the PPS backbone can interact with the thiol sulfur of 2-mercaptopyridine through soft van der Waals and polarizable sulfur–sulfur interactions. These proximity effects create localized zones of interaction that may subtly influence chain alignment and packing density. In parallel, the pyridine nitrogen can engage in electron donor–acceptor interactions with electron-rich regions along the PPS chain, forming directional pathways that facilitate electronic communication between polymer segments [9].

Together, these sulfur–sulfur and sulfur–nitrogen interactions generate a cooperative network of transient molecular associations. This network is predicted to guide conformational adjustments and local electronic redistribution, enabling the polymer to accommodate the modifier without compromising its inherent thermal or mechanical stability. Such a mechanism represents a strategic approach to molecular-level tuning, where small molecule incorporation produces significant functional enhancement with minimal structural perturbation.

2.4 Expected Impact on Polymer Micro-Environment

The inclusion of 2-mercaptopyridine is anticipated to result in a profound influence on the PPS micro-environment. At the molecular scale, heteroatom interactions induce localized electronic redistribution along the polymer backbone, potentially altering charge density and enhancing interchain electronic communication. These modifications may increase the polymer's responsiveness to external stimuli, such as electromagnetic fields or thermal stress.

In addition to electronic effects, 2-mercaptopyridine incorporation may promote subtle conformational rearrangements and changes in chain packing. Minor adjustments in torsional angles or local chain alignment can create microdomains of enhanced stability and functionality. The synergistic effect of electronic redistribution and framework reorganization establishes a direct structure–function correlation, providing a pathway for rational design of high-performance polymers with tunable properties. By strategically exploiting heteroatom-rich molecular modifiers, it becomes possible to achieve controlled functional enhancement while retaining the hallmark stability of PPS [9].

3. STRUCTURAL MODIFICATION INDUCED BY 2-MERCAPTOPYRIDINE

3.1 Changes in Molecular Organization

Incorporation of 2-mercaptopyridine into the PPS matrix leads to noticeable changes in polymer chain alignment and packing. Pristine PPS exhibits semi-crystalline domains with relatively uniform chain spacing, which contributes to its high thermal and mechanical stability. However, the introduction of heteroatom-rich modifiers such as 2-mercaptopyridine creates localized regions of interaction that perturb the regular packing arrangement [10]. The sulfur atoms of the polymer backbone interact with the thiol group of 2-mercaptopyridine, resulting in subtle shifts in interchain distances and alignment. These localized modifications do not disrupt the polymer's overall crystallinity but rather introduce microheterogeneity that enhances electronic communication pathways and functional responsiveness.

The alteration in intermolecular distances can also influence van der Waals and π–π stacking interactions between aromatic units. These changes can promote adaptive rearrangements of polymer chains, allowing the matrix to accommodate the modifier while maintaining structural integrity. Such modulation of chain packing is essential for tuning functional properties such as electronic polarizability and optical response, which are sensitive to local molecular organization.

3.2 Influence on Backbone Conformation

Although PPS possesses a rigid aromatic backbone, localized conformational adjustments are possible in regions interacting with 2-mercaptopyridine. The presence of the modifier can induce minor torsional distortions in phenyl rings or slight bending along the polymer chain [11]. These adjustments increase local flexibility without compromising the overall backbone rigidity, creating a balance between structural stability and functional adaptability.

By modulating local conformations, 2-mercaptopyridine enables enhanced spatial overlap between electronic orbitals of adjacent polymer segments. This facilitates charge delocalization and improved electronic communication, which is crucial for high-performance polymer applications. The interplay between chain rigidity and localized flexibility illustrates the importance of controlled molecular interactions in achieving targeted functional enhancement.

3.3 Role of Heteroatom Interactions

Heteroatom interactions play a central role in guiding the structural evolution of PPS upon modification. The sulfur atoms in the polymer backbone can form soft, non-covalent interactions with the thiol group of 2-mercaptopyridine, resulting in preferential binding sites that stabilize specific molecular arrangements [12]. These sulfur–sulfur interactions influence local packing and provide transient anchoring points for polymer chains, contributing to enhanced coherence within the microstructure.

In addition, the nitrogen atom of the pyridine ring participates in donor–acceptor interactions with electron-rich regions along the PPS backbone. This directional coupling helps align polymer segments and reinforces intermolecular cohesion. The cooperative effect of sulfur and nitrogen interactions establishes a heteroatom-assisted interaction network that governs both local chain organization and electronic distribution, thereby linking structural modification directly to functional outcomes.

3.4 Structural Stability Considerations

Despite the induced molecular reorganization, PPS retains its intrinsic thermal and mechanical stability upon 2-mercaptopyridine incorporation. The non-covalent nature of the interactions ensures that the primary aromatic backbone remains intact while secondary structural features adapt to accommodate the modifier [13]. These interaction-driven stabilization effects reduce structural fluctuations, promote long-range coherence, and provide reinforcement to semi-crystalline domains.

The establishment of a cooperative heteroatom interaction network contributes to enhanced resistance against external perturbations, such as thermal stress or mechanical deformation. By simultaneously modulating local chain flexibility and preserving overall rigidity, 2-mercaptopyridine enhances both the structural and functional robustness of PPS. These findings highlight the critical role of controlled molecular interactions in designing high-performance polymers with tunable properties.

4. Electronic Redistribution and Functional Response

4.1 Modification of Electronic Density Distribution

The incorporation of 2-mercaptopyridine into the PPS matrix significantly influences the distribution of electronic density along the polymer backbone. In pristine PPS, electron delocalization is primarily confined to the aromatic units and sulfur linkages, providing moderate electronic communication across chains. Upon inclusion of 2-mercaptopyridine, heteroatom proximity induces localized perturbations, leading to both electron localization near interaction sites and enhanced delocalization in adjacent segments [14].

The thiol sulfur interacts with backbone sulfur atoms, creating regions of electron density accumulation, while the pyridine nitrogen can act as a localized electron donor, facilitating redistribution across the polymer chain. This dual modulation allows fine-tuning of electron density profiles, potentially enhancing functional responsiveness to external stimuli such as electromagnetic fields or applied potentials.

4.2 Polymer–Modifier Electronic Communication

2-Mercaptopyridine acts as an effective mediator of electronic communication within the PPS framework. The cooperative effect of sulfur–sulfur and nitrogen–sulfur interactions establishes transient pathways for charge transfer between polymer chains and modifier molecules [15]. These pathways facilitate partial delocalization of charge carriers, effectively increasing the electronic connectivity of the matrix without covalent alteration of the polymer backbone.

This type of cooperative electronic behavior enhances the polymer’s ability to respond to external perturbations and supports emergent functional phenomena such as improved conductivity, nonlinear optical response, or charge storage capabilities. The modification thus enables a controlled tuning of polymer electronic properties at the molecular level, guided by strategic heteroatom placement.

4.3 Influence on Electronic Response Characteristics

The electronic response of PPS is highly sensitive to localized structural reorganization induced by 2-mercaptopyridine. Changes in chain packing and backbone conformation influence orbital overlap, thereby affecting the polymer’s polarizability and electronic transitions [16]. The presence of heteroatom interactions enhances this sensitivity, providing a means to modulate electronic behavior in a predictable manner.

This tunability allows the material to achieve desired functional characteristics, such as adjustable electronic conductivity, optical absorption, or dielectric properties. By varying the concentration or distribution of the modifier, the electronic response can be systematically optimized, demonstrating the potential for molecular-level design strategies in high-performance polymers.

4.4 Structure-Dependent Functional Evolution

The observed functional enhancements are directly correlated with structural modifications at the molecular level. Localized backbone adjustments, chain alignment variations, and heteroatom-mediated interactions collectively determine how electronic density is redistributed and how functional pathways develop [17].

This structure-dependent evolution enables precise molecular-scale control of material response. For example, regions of enhanced electron delocalization correspond to zones of increased optical or electronic activity, while stabilized interaction networks promote sustained functional performance under stress. Consequently, the combination of structural tuning and electronic modulation defines a coherent framework for designing high-performance, heteroatom-modified polymers with tailored properties suitable for advanced applications in electronics, photonics, and energy systems.

5.INTERMOLECULAR INTERACTION-DRIVEN STABILITY ENHANCEMENT

5.1 Contribution of Sulfur-Containing Motifs

Sulfur atoms present in both the PPS backbone and the thiol group of 2-mercaptopyridine contribute significantly to the formation of non-covalent interaction networks. These interactions, often described as “soft-atom” contacts, create localized zones of enhanced interaction density, which stabilize specific chain arrangements without altering the primary structure of the polymer [18]. Such soft-atom interactions are particularly effective in reinforcing semi-crystalline domains, as they promote intermolecular cohesion through polarizable electron clouds.

Additionally, the sulfur-mediated interactions facilitate subtle adjustments in chain alignment, which can enhance orbital overlap between adjacent polymer segments. These structural refinements provide a micro-environment conducive to electronic communication and functional responsiveness, demonstrating the dual role of sulfur motifs in structural and electronic stabilization.

5.2 Nitrogen-Assisted Interaction Networks

The pyridine nitrogen atom of 2-mercaptopyridine introduces directional, donor–acceptor interactions within the polymer matrix. These interactions act as localized anchoring points, guiding the orientation of polymer chains and enhancing intermolecular coherence [19]. The nitrogen-mediated interactions are particularly important in maintaining long-range structural order while accommodating molecular modifiers.

By stabilizing specific chain conformations and promoting preferred orientations, nitrogen-assisted networks complement sulfur-mediated interactions. This dual functionality allows for fine control of polymer microstructure, supporting both stability and functional performance under mechanical, thermal, or chemical stress.

5.3 Synergistic Effect of Dual Heteroatoms

The cooperative action of sulfur and nitrogen heteroatoms generates a synergistic stabilization effect. Sulfur–sulfur and sulfur–nitrogen interactions work in tandem to reduce local structural fluctuations, creating a network of transient but robust connections throughout the polymer matrix [20]. This synergy enhances the resilience of the polymer, allowing it to maintain both its structural and functional integrity in challenging operational conditions.

Such dual-heteroatom interaction networks also influence the polymer’s electronic landscape by maintaining optimal orbital overlap and facilitating charge delocalization. The simultaneous structural and electronic stabilization underscores the importance of heteroatom complementarity in high-performance polymer design.

5.4 Implications for Long-Term Material Performance

The establishment of stable, heteroatom-assisted interaction networks has direct implications for the long-term performance of PPS-based systems. Structurally, these networks contribute to improved rigidity, reduced chain mobility, and sustained microstructural coherence under stress. Functionally, they support consistent electronic and optical behavior, ensuring reliability in applications such as electronics, photonics, and energy storage [21].

Overall, the combination of sulfur- and nitrogen-mediated stabilization enhances both robustness and functional consistency, demonstrating that controlled molecular interactions can be leveraged to design polymers with predictable, tunable, and long-lasting properties.

6. STRUCTURE–FUNCTION RELATIONSHIP ANALYSIS

6.1 Correlation Between Molecular Arrangement and Function

The functional properties of PPS are closely tied to its molecular arrangement. In the unmodified polymer, semi-crystalline domains and ordered chain packing define the primary pathways for electronic and thermal transport. Upon incorporation of 2-mercaptopyridine, localized heteroatom interactions induce subtle reorganization in chain alignment and packing density [22]. These structural modifications create enhanced electronic pathways, enabling more efficient charge transport and improved responsiveness to external stimuli.

Such correlations indicate that even minor changes in molecular arrangement can have disproportionate effects on functional performance. The formation of well-aligned interaction networks facilitates cooperative electronic behavior, where multiple polymer segments participate in delocalized charge transfer. Consequently, molecular-level design strategies can be employed to optimize functional responses by controlling chain packing and heteroatom placement within the polymer matrix.

6.2 Functional Sensitivity to Molecular Modification

PPS exhibits notable sensitivity to molecular modifications introduced by 2-mercaptopyridine. The degree of property modulation depends on the density and distribution of heteroatom interactions, which govern electronic redistribution and local conformational flexibility [23]. By varying the concentration of the modifier or adjusting processing conditions, specific functional parameters—such as polarizability, optical response, or conductivity—can be tuned in a controlled manner.

This tunability underscores the potential of targeted molecular design in high-performance polymer systems. Controlled introduction of small molecules enables precise adjustment of electronic, mechanical, and optical properties without compromising thermal stability. The ability to modulate function predictably provides a foundation for engineering polymers for advanced applications, including photonics, electronics, and energy storage.

6.3 Comparative Insight with Unmodified PPS

Comparison with unmodified PPS highlights the distinct behavior induced by 2-mercaptopyridine. While pristine PPS demonstrates stable structural and electronic properties, its functional response is limited by rigid chain packing and moderate electronic delocalization. Modification with 2-mercaptopyridine introduces heteroatom-mediated interaction networks that enhance both structural adaptability and electronic connectivity [24].

These differences manifest in improved electronic communication, enhanced charge delocalization, and greater sensitivity to external stimuli. Such performance differentiation emphasizes the importance of molecular-level modification in achieving tunable and responsive high-performance polymers. The study demonstrates that minor adjustments at the molecular scale can significantly expand the functional capabilities of otherwise rigid polymer frameworks.

6.4 Design Principles Derived from Observations

Several key principles emerge from the structure–function analysis. First, the placement and density of heteroatoms within a polymer matrix critically influence both structural organization and functional responsiveness. Second, cooperative interactions between dual heteroatoms (sulfur and nitrogen) are more effective in promoting structural stability and electronic communication than single-atom modifications. Third, controlled local conformational flexibility enables enhanced electronic pathways without compromising overall polymer rigidity [25].

These insights provide actionable guidelines for polymer design: selection of heteroatom-rich modifiers, optimization of their spatial distribution, and tuning of processing conditions can collectively produce high-performance materials with predictable and tunable properties. By establishing a direct link between structural reorganization and functional outcomes, this approach underscores the importance of molecular-scale engineering in developing next-generation functional polymers.

7. IMPLICATIONS FOR ADVANCED FUNCTIONAL MATERIALS

7.1 Relevance to Electronic and Functional Applications

The incorporation of 2-mercaptopyridine into PPS demonstrates clear potential for advancing polymer-based electronic and functional materials. Enhanced electronic communication, facilitated by heteroatom-mediated interactions, supports improved charge transport and polarizability, which are critical for applications in flexible electronics, sensors, and optoelectronic devices [26]. Additionally, the tunable structural and functional properties enable the design of functional coatings with controlled electronic, optical, or thermal characteristics, extending the applicability of PPS-based systems to diverse device architectures.

The ability to modulate electronic density and chain organization at the molecular level provides a unique advantage in tailoring polymer behavior for specific device requirements. By exploiting structure–function relationships established in the present study, polymer-based materials can be engineered for enhanced performance while maintaining intrinsic thermal and mechanical robustness.

7.2 Advantages of Small-Molecule Modification Strategy

The use of small, heteroatom-rich molecules like 2-mercaptopyridine offers several practical benefits for polymer modification. This strategy is relatively simple and versatile, allowing targeted tuning of electronic and structural properties without the need for complex chemical synthesis or backbone modification [27]. Moreover, the approach is inherently scalable; small-molecule modifiers can be introduced during polymer processing or post-synthesis functionalization, providing flexibility for large-scale manufacturing of functional polymer systems.

Importantly, this method allows precise control over the degree of functionalization, enabling systematic optimization of properties such as conductivity, optical response, and chemical stability. The combination of simplicity, versatility, and scalability positions small-molecule modification as an attractive route for the development of high-performance functional polymers.

7.3 Extension to Other Polymer Systems

The insights gained from PPS modification are broadly applicable to other high-performance polymer systems. Heteroatom-rich small molecules can be used to tune structural and functional properties in polymers with aromatic backbones, conjugated systems, or sulfur-containing linkages [28]. This general applicability opens avenues for designing next-generation materials with tailored properties for electronics, photonics, energy storage, and smart coatings.

Future material design can leverage the structure–function correlations and interaction mechanisms established in the present work to achieve molecularly precise control over polymer performance. By extending this strategy across diverse polymer platforms, it is possible to develop a new class of functional materials that combine tunable electronic behavior with structural stability and long-term reliability.

8. CONCLUSIONS

The present study demonstrates that the incorporation of 2-mercaptopyridine into polyphenylene sulfide (PPS) induces significant structural reorganization and functional enhancement at the molecular level. Heteroatom-mediated interactions, including sulfur–sulfur and sulfur–nitrogen proximity effects, result in localized modifications in chain alignment, backbone conformation, and electronic density distribution, which collectively improve electronic communication, polarizability, and responsiveness of the polymer matrix [29]. This work provides novel molecular-level insight into the cooperative role of dual heteroatoms, elucidating how controlled modifications can enhance both structural stability and electronic functionality, thereby clarifying the fundamental structure–function relationship in high-performance polymers [30]. The findings also establish a framework for rational polymer design, highlighting the potential of heteroatom-rich small molecules to tune functional properties predictably. Building on these insights, future research can explore alternative heteroatom-rich modifiers, optimize their concentration and spatial distribution, and extend the strategy to other high-performance polymers, enabling the development of next-generation functional materials with tunable properties, application-specific performance, and long-term reliability in electronics, photonics, and energy systems [31].

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