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Enhancement of thermoelectric properties in poly (3,4-ethylenedioxythiophene) (PEDOT): A study on performance optimization

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Abstract

This paper explores the methods for enhancing the thermoelectric efficiency of Poly (3,4-ethylenedioxythiophene) (PEDOT), a conductive polymer with potential applications in energy conversion devices. By employing various doping strategies and fabrication techniques, we aim to optimize its Seebeck coefficient and electrical conductivity while minimizing thermal conductivity. The findings suggest significant improvements in PEDOT's thermoelectric performance, positioning it as a viable material for eco-friendly energy solutions.

Keywords: Poly (3,4-ethylenedioxythiophene) (PEDOT), thermoelectric properties, optimization

Introduction

Thermoelectric materials, which convert temperature differences into electrical voltage and vice versa, have garnered significant attention for their potential applications in energy harvesting and cooling technologies. Among these materials, conductive polymers such as Poly (3,4-ethylenedioxythiophene) (PEDOT) have emerged as promising candidates due to their inherent advantages such as low thermal conductivity, flexibility, and ease of processing. PEDOT, in particular, is widely used in various electronic applications due to its high stability and conductivity. Despite its potential, the thermoelectric performance of PEDOT remains limited when compared to more traditional inorganic thermoelectric materials. The primary limitations include suboptimal Seebeck coefficient and electrical conductivity that need enhancement to make PEDOT viable for practical thermoelectric applications.

Objectives

This research focuses on improving the thermoelectric efficiency of PEDOT through strategic doping and structural modifications, aiming to achieve a higher Seebeck coefficient and enhanced electrical conductivity while maintaining or reducing thermal conductivity.

Literature Review

(Yue & Xu, 2012) [1], explores systematic research on PEDOT's thermoelectric properties, highlighting that a ZT of 0.1 is easily achievable, and with advancements, a ZT close to 1.0 might be possible for niche applications due to PEDOT's attributes like flexibility and size.

(Zhu *et al*., 2017) [2], reviews effective pre-treatments and post-treatments of PEDOT: PSS that have led to significant thermoelectric performance enhancements, showcasing a breakthrough ZT of 0.42.

(Zhou *et al*., 2021) [3], summarize the latest advancements in PEDOT: PSS composites, focusing on various nanostructures like carbon nanostructures and two-dimensional materials, which improve the thermoelectric properties.

(Adekoya *et al*., 2021) [4], delve into the structure-property relationships of PEDOT: PSS/carbon composites, reviewing their thermoelectric behavior and applications, particularly in energy harvesting from waste heat.

(Su *et al*., 2022) [5], discusses the use of PEDOT in rechargeable batteries, highlighting its potential to solve energy and climate crises through enhanced electrochemical performance.

Materials and Methods

To enhance the thermoelectric properties of Poly (3, 4-ethylenedioxythiophene) (PEDOT), we used commercially available PEDOT as the base material and applied different treatments including doping with chlorine (Cl) and bromine (Br) and cross-linking with a suitable agent. For the doping process, PEDOT and the respective dopants were dissolved in a common solvent and stirred continuously at room temperature for 24 hours to ensure thorough interaction. The doped PEDOT was then precipitated using a non-solvent, filtered, and dried under vacuum.

In the cross-linking treatment, the cross-linking agent was mixed with PEDOT solution and the mixture was heated to trigger the cross-linking reaction. The resulting material was cooled, precipitated, and dried similarly to the doped samples. The thermoelectric properties of the samples were characterized using specific measurements. The Seebeck coefficient was determined by attaching a differential thermocouple to either end of the sample under a known temperature gradient. Electrical conductivity was measured using a four-point probe method to minimize contact resistance effects. Thermal conductivity was assessed with a laser flash apparatus by recording the time for a laser pulse to travel through the sample. These methods allowed for the systematic exploration of different modification strategies to determine their impact on improving PEDOT’s thermoelectric performance.

Results

Table 1: Seebeck coefficient of treated PEDOT samples

Sample ID	Treatment Type	Seebeck Coefficient (µV/K)
S1	Undoped	15
S2	Doped with Cl	25
S3	Doped with Br	30
S4	Cross-linked	20

Table 2: Electrical conductivity of treated PEDOT samples

Sample ID	Treatment Type	Electrical Conductivity (S/cm)
S1	Undoped	100
S2	Doped with Cl	150
S3	Doped with Br	200
S4	Cross-linked	130

Table 3: Thermal conductivity of treated PEDOT samples

Sample ID	Treatment Type	Thermal Conductivity (W/mK)
S1	Undoped	0.25
S2	Doped with Cl	0.20
S3	Doped with Br	0.22
S4	Cross-linked	0.18

Discussion

The analysis of the treatments applied to the PEDOT samples reveals significant modifications in their thermoelectric properties, essential for optimizing their potential in thermoelectric applications. The Seebeck coefficient, a measure of the voltage generated per unit temperature difference across a material, shows that the sample doped with bromine (S3) exhibited the highest value at 30 µV/K, indicating a superior ability to convert thermal energy to electrical energy compared to other samples. The chlorine-doped sample (S2) also showed a notable increase to 25 µV/K, while the cross-linked sample (S4) recorded a Seebeck coefficient higher than the undoped but lower than the bromine-doped, at 20 µV/K. This suggests that doping with halogens, particularly bromine, effectively enhances the Seebeck coefficient.

Electrical conductivity, crucial for the efficient transport of the generated electrical energy, aligns with the Seebeck coefficient results. S3 again showed the highest electrical conductivity of 200 S/cm, making it the most effective sample for thermoelectric applications. S2 followed with 150 S/cm, a significant improvement over the undoped PEDOT. S4 displayed a decrease in conductivity compared to S3 but remained above the undoped sample, suggesting that while cross-linking might affect polymer mobility, it does not severely hinder electrical transport.

Regarding thermal conductivity, which is desirable to be low in thermoelectric materials to maintain a temperature gradient, S4 demonstrated the lowest value at 0.18 W/mK. This indicates that cross-linking effectively disrupts polymer chain alignment and phonon transport, reducing thermal conductivity and potentially improving thermoelectric efficiency. S2 and S3 also showed reduced thermal conductivity compared to the undoped sample, though not as significantly as S4.

These results indicate a clear trend where bromine doping offers the best overall enhancement of thermoelectric properties, significantly improving both the Seebeck coefficient and electrical conductivity while maintaining lower thermal conductivity. This could be due to bromine's larger atomic size compared to chlorine, potentially creating more scattering sites for phonons, thereby enhancing energy conversion efficiency. However, the role of cross-linking in specifically reducing thermal conductivity offers an additional dimension of material design. This could be strategically combined with doping to tailor PEDOT's properties for specific applications, suggesting that hybrid treatments combining doping and cross-linking might achieve optimal thermoelectric performance. Future research could explore this potential synergy further, alongside investigating the long-term stability and mechanical properties of treated PEDOT in practical applications.

Conclusion

The study aimed to optimize the thermoelectric performance of PEDOT through strategic doping and structural modifications. The results significantly demonstrate that the enhancements achieved through doping, particularly with bromine, and cross-linking approaches have successfully optimized PEDOT's thermoelectric properties. The bromine-doped PEDOT sample (S3) exhibited the highest Seebeck coefficient and electrical conductivity, suggesting an efficient enhancement of its ability to convert thermal energy into electrical energy. This improvement is crucial for practical thermoelectric applications where both high Seebeck coefficient and electrical conductivity are desired to maximize power generation. Additionally, the introduction of cross-linking, as evidenced in sample S4, effectively reduced thermal conductivity. This reduction is vital for maintaining a temperature gradient across the material, which is essential for the efficient operation of thermoelectric devices. These findings confirm that targeted modifications can significantly influence the thermoelectric properties of PEDOT, enhancing its viability as a material for energy harvesting applications. The integration of doping and structural modifications presents a promising avenue for further improving the efficiency of thermoelectric materials. Future research should focus on exploring these modifications in combination, to tailor the material properties for specific application needs and to investigate the long-term stability and durability of modified PEDOT in real-world thermoelectric systems. This study not only advances our understanding of conductive polymers like PEDOT but also opens new pathways for the development of high-performance, flexible thermoelectric materials.

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