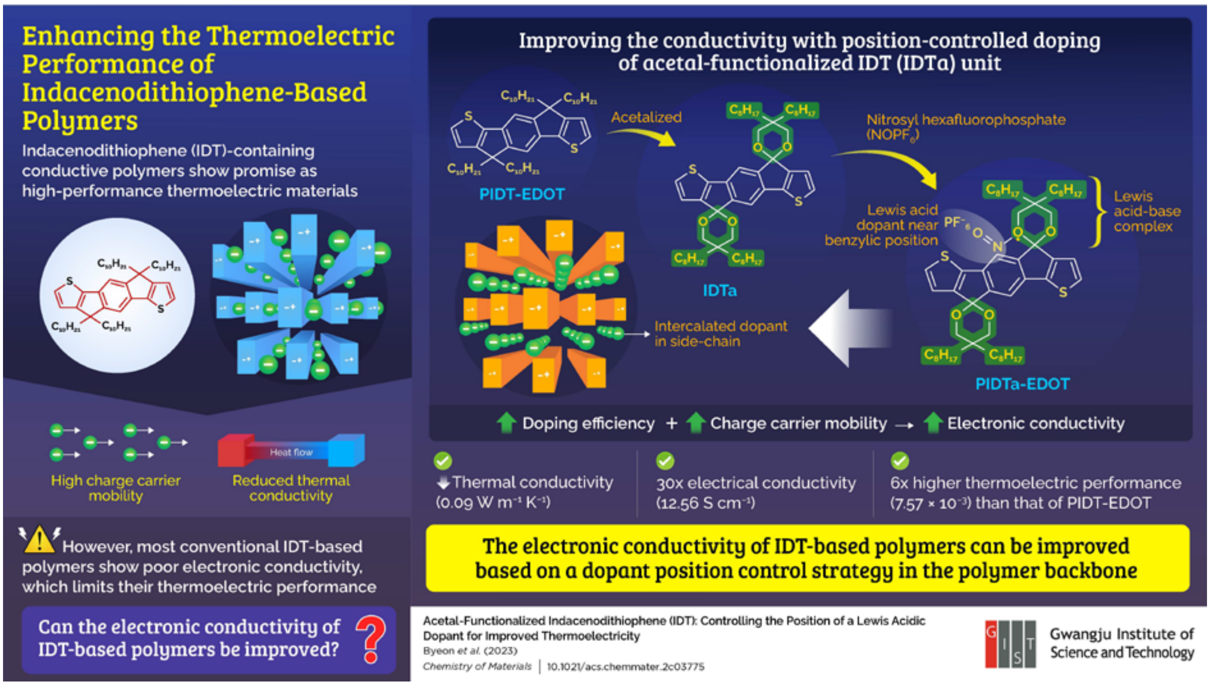
PRESS RELEASE

Gwangju Institute of Science and Technology Researchers Enhance Thermoelectricity with Guided Impurity Position Control

Scientists devise a position-controlled doping strategy to improve the thermoelectric performance of indacenodithiophene-based polymer

High charge carrier mobility and low thermal conductivity of indacenodithiophene (IDT)-based polymers make them ideal candidates for thermoelectric materials. However, they suffer from low electric conductivity, a prerequisite for high thermoelectric performance. In a new study, researchers from Korea show that a strategy based on controlling dopant position near the IDT polymer skeleton can significantly improve the electric conductivity and thermoelectric performance of these systems.



Title: New strategy for improving the thermoelectric performance of IDT-based polymers.

Caption: A new approach developed by researchers from GIST, Korea guides a Lewis-acid dopant to the sidechains of the polymer backbone by acetal functionalizing the IDT-based polymer prior to the doping, resulting in an enhanced electronic conductivity and thermoelectric performance.

Credit: Sukwon Hong from Gwangju Institute of Science and Technology

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Thermoelectric materials, substances that convert temperature difference into electricity, find a multitude of applications involving the conversion of waste heat into useful electrical energy. However, they often need to rely on heavy rare earth elements for efficient thermoelectric conversion. This, unfortunately, makes them expensive and environmentally hazardous. In recent years, conjugated polymer-based material has received attention as an environmentally benign alternative to the conventional rare earth metal-based thermoelectric materials.

Owing to their high charge carrier mobility in the amorphous state, IDT-containing conductive polymers have the potential to reduce thermal conductivity while keeping their electronic conductivity intact. Unfortunately, these polymers suffer from low electronic conductivity, limiting our ability to synthesize high-performance thermoelectric materials from IDT-based polymers.

A team of researchers led by Prof. Sukwon Hong Gwangju Institute of Science and Technology in Korea have now found a solution to the problem. Equipped with their understanding of plausible reasons for the observed low conductivity, the team designed a novel strategy for developing an IDT-based polymer with improved thermoelectric performance based on dopant (impurity) position controlling within an acetal-functionalized IDT (IDTa) polymer. Their study was made available online on March 2, 2023 and was published in Volume 35, Issue 5 of the journal *Chemistry of Materials* on March 14, 2023.

The team chose PIDT-EDOT, a copolymer of IDT and then acetal-functionalized it to form PIDTa-EDOT. Next, they synthesized a Lewis-acid base complex by introducing nitrosyl hexafluorophosphate ($NOPF_6$), a Lewis acidic dopant into the IDTa component. The addition of the acetal group was crucial, since it directed the dopant next to the benzylic position of the polymer skeleton, facilitating the desired dopant position control.

"We showed that the low conductivity of conventional IDT results from their non-polar side chains, which cause the dopant to be located between the polymer chains (backbone) instead of at the side chains. This, in turn, impedes charge transfer. Accordingly, we proposed a strategy that would allow us to place the dopant near the sidechains of the polymer backbone," explains Prof. Hong, when asked about the motivation behind the study.

Upon testing the PIDTa-EDOT polymer, the researchers observed an improved doping efficiency, condensed π−π stacking, and reduced grain size. These, in turn, imparted a low thermal conductivity of 0.09 $W\ m^{-1}\ K^{-1}$ on one hand and 30 times higher electronic conductivity on the other. As a result, the PIDTa-EDOT polymer demonstrated a 6-fold improvement in thermoelectric performance compared to that of pristine PIDT-EDOT polymer.

The study thus presents a new approach to synthesizing IDT-based polymers that simultaneously exhibit low thermal conductivity and high electronic conductivity, a prerequisite for developing efficient thermoelectric materials and thermoelectric conversion technology. "*Improved thermoelectric materials could lead to more efficient electricity generation from the waste heat released in industrial processes or even from the human body. This, in turn, could reduce energy consumption and make solar power more practical and cost-effective,"* concludes an optimistic Prof. Hong.

Reference

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About the Gwangju Institute of Science and Technology (GIST)

The Gwangju Institute of Science and Technology (GIST) is a research-oriented university situated in Gwangju, South Korea. Founded in 1993, GIST has become one of the most prestigious schools in South Korea. The university aims to create a strong research environment to spur advancements in science and technology and to promote collaboration between international and domestic research programs. With its motto of "A Proud Creator of Future Science and Technology," GIST has consistently received one of the highest university rankings in Korea.

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About the author

Sukwon Hong is a Professor of Chemistry at Gwangju Institute of Science and Technology (GIST), Korea. He received his PhD in Chemistry from Northwestern University, USA. Before joining GIST, he worked as assistant professor at the University of Florida till 2012. His current areas of research include development of organometallic catalyst for asymmetric reaction, ethenolysis, CO_2 chemistry, and photochemistry. The Hong group at GIST has been working on developing functional molecules for energy conversion technology, including solar cells and thermoelectric materials.