

論文 / 著書情報
Article / Book Information

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論文要旨

THESIS SUMMARY

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要旨 (英文 800 語程度)

Thesis Summary (approx.800 English Words)

Water scarcity remains one of the most pressing global challenges, exacerbated by population growth, urbanization, and industrial pollution. The increasing demand for clean water necessitates the development of energy-efficient and environmentally sustainable water purification technologies. Conventional methods, such as reverse osmosis and chemical treatments, are highly energy-intensive and generate hazardous byproducts, making them unsuitable for widespread implementation in remote or resource-limited regions. Solar steam generation (SSG) has emerged as a promising alternative for water purification, utilizing solar energy to drive the evaporation and condensation processes. Unlike conventional techniques, SSG operates without the need for extensive infrastructure or high energy input, making it a viable solution for decentralized water treatment. Recent advancements in photothermal materials (PTMs) have significantly improved SSG efficiency, enabling higher evaporation rates and better energy utilization. This thesis explores the development and application of donor-acceptor molecules and polymers as PTMs for SSG, focusing on their synthesis, functionalization, and performance in solar-driven water purification.

In Chapter 1, it is described that the efficiency of solar steam generation (SSG) systems is primarily governed by three key factors: light absorption efficiency, photothermal conversion efficiency, and vaporization efficiency. The ability of a material to effectively absorb solar radiation is critical for determining the overall performance of an SSG device. Materials with high light absorption coefficients can convert a larger fraction of incident solar energy into thermal energy, enhancing photothermal performance. Photothermal conversion efficiency refers to how effectively absorbed solar energy is converted into heat. To maximize this efficiency, materials must exhibit low photoluminescence and minimal energy loss, ensuring that most captured energy contributes to the heating process rather than being dissipated as light. Vaporization efficiency plays a crucial role in the transformation of liquid water into steam and is significantly influenced by the design of the SSG device, particularly in terms of water transport and evaporation dynamics.

To enhance the photothermal properties of organic semiconductors for SSG applications, Chapter 2 focuses on the functionalization of dithienoindacenodithiophene (DTIDT) molecules. DTIDT is widely recognized for its excellent optoelectronic properties; however,

its high photoluminescence quantum yield limits its effectiveness as a PTM due to substantial energy loss in the form of emitted light rather than heat. To address this limitation, the [2+2] cycloaddition-retroelectrocyclization (CA-RE) reaction was employed to modify DTIDT's molecular structure, thereby enhancing its photothermal properties for SSG applications. The CA-RE reaction, a highly efficient and selective click reaction, involves a two-step transformation: cycloaddition, forming a four-membered cyclobutene ring, followed by retroelectrocyclization, which opens the ring to yield a new conjugated system. This reaction significantly alters DTIDT's molecular structure, converting its originally planar configuration into a non-planar form, which enhances intramolecular charge transfer and broadens its optical absorption. These modifications reduce photoluminescence quantum yield and increase solar-to-heat conversion efficiency, making DTIDT derivatives highly effective PTMs. To further optimize the photothermal response, three different electron acceptors—tetracyanoethylene (TCNE), tetracyanoquinodimethane (TCNQ), and tetrafluoro-tetracyanoquinodimethane (F4TCNQ) were incorporated through [2+2] CA-RE reactions. To evaluate their SSG potential, DTIDT derivatives were drop cast on filter paper as Janus membranes consisting of a hydrophobic upper layer and a hydrophilic lower layer. The hydrophobic layer minimized heat loss and prevented excessive water accumulation, while the hydrophilic layer ensured continuous water transport through capillary action. Under simulated sunlight, DTIDT, DTIDT-TCNE, DTIDT-TCNQ, and DTIDT-F4TCNQ exhibited SSG efficiencies of 57.3%, 61.3%, 72.5%, and 78.3%, respectively.

In addition to small-molecule functionalization, Chapter 3 also explores the use of vinylene-linked naphthalenediimide (vNDI)-based dual-acceptor copolymers as PTMs. Naphthalenediimide (NDI) is a widely used electron acceptor in donor-acceptor polymers and is valued for its strong electron-withdrawing properties, thermal stability, and high photochemical robustness. The incorporation of a dual-acceptor strategy enhances light absorption, charge generation, and photothermal performance, making these materials promising candidates for SSG. To investigate this approach, four vNDI-based polymers were synthesized with different acceptor units: benzothiadiazole (S), benzotriazole (N), triazolobenzothiadiazole (NS), and benzobistriazole (NN). Structural modifications included vinylene bridging for enhanced charge transport, selenophene spacers to alleviate steric hindrance and improve charge transfer, and silane side chains for better polymer solubility and film formation. These modifications collectively improved the polymers' optoelectronic and photothermal properties. Similar to the DTIDT derivatives, these polymers were integrated into Janus photothermal membranes and tested for their SSG performance. Among them, vNDI-NS exhibited the highest efficiency, achieving a solar-to-vapor conversion efficiency of 58.3%. While the performance was lower than that of DTIDT-F4TCNQ, this study highlighted the potential of dual-acceptor polymer engineering for photothermal applications.

This thesis demonstrates that donor-acceptor molecular engineering is an effective strategy for optimizing PTMs for SSG applications. The findings indicate that post-functionalization via the [2+2] CA-RE reaction significantly enhances the photothermal efficiency of small molecules by altering the molecular structure and charge transfer properties. Furthermore, the use of dual-acceptor NDI-based polymers with vinylene bridges and selenophene spacers results in improved charge transport and broadened optical absorption spectra, contributing to enhanced solar-to-heat conversion efficiency. The incorporation of Janus membrane architectures plays a critical role in thermal management and water transport, ultimately improving solar-to-vapor conversion efficiencies in both small-molecule and polymer-based PTMs. Future research should focus on further optimizing donor-acceptor interactions, improving scalability, and integrating these materials into real-world solar water purification systems. The findings presented in this thesis contribute to the development of high-efficiency, solar-driven water purification technologies with broad implications for sustainable water resource management.

備考：論文要旨は、和文 2000 字と英文 300 語を 1 部ずつ提出するか、もしくは英文 800 語を 1 部提出してください。

Note: Thesis Summary should be submitted in either a copy of 2000 Japanese Characters and 300 Words (English) or 1 copy of 800 Words (English).

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