Nanotechnology, Molecular electronics, Organic electronics

Development of molecular wires towards efficient intramolecular hopping transport

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Abstract

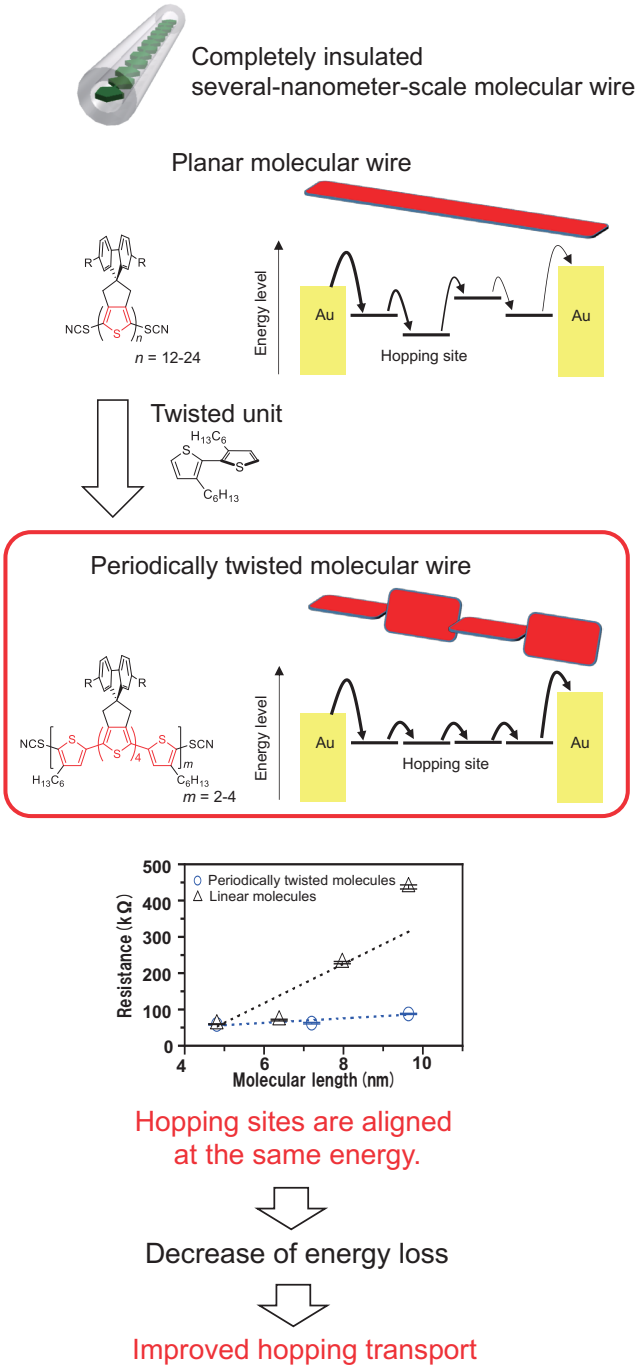
The development of several-nanometer-scale π-conjugated molecules for efficient intramolecular hopping charge transport remains a significant challenge. To construct localized electronic structures at the same energy in a molecule, a series of molecular wire, with lengths up to 10 nm and periodically twisted structures, was synthesized. Single-molecule conductance measurements of the twisted molecules revealed resistances lower than those of planar molecules. This study provides a rational molecular design to improve the intramolecular hopping charge transport.

Background & Results

Elucidating the nature of long-range intramolecular charge transport in π-conjugated systems is of considerable importance for a wide range of scientific fields, from chemistry to materials science and physics. In contrast to coherent tunneling charge transport, which governs charge transport over a short distance, the establishment of design principles for molecules with efficient hopping transport, which governs charge transport over a long distance, remains elusive due to difficulties in the molecular design and synthesis of several-nanometer-scale π-conjugated systems. Under this situation, we synthesized a series of several-nanometer-scale oligothiophenes with periodically twisted structures and localized conjugation. Each conjugation unit serves as a hopping site at the same energy, which should result in more effective hopping transport than in molecules without periodically localized conjugation. As expected, single-molecule electrical conductance measurements using the scanning tunneling microscope–break junction technique revealed that the resistance of the newly synthesized molecules were lower than those of the linear oligothiophenes that we had reported previously.

Significance of the research and Future perspective

In this study, we successfully designed “uniformed” intramolecular hopping sites by the modification of molecular structures and improved the long-range intramolecular hopping charge transport. These findings give significant new insights into the field of molecule-based electronics in terms of unveiling a general design principle for organic materials to improve their electrical conduction.



Patent	Japanese Patent Application No. 2005-065947 Japanese Unexamined Patent Publication No. 2006-248945, Japanese Patent No. 4505568
Treatise	Ie, Yutaka; Tada, Hirokazu; Aso, Yoshio et al. Highly Planar and Completely Insulated Oligothiophenes: Effects of π-Conjugation on Hopping Charge Transport J. Phys. Chem. Lett. 10 2019; 3197-3204. doi: 10.1021/acs.jpclett.9b00747 Ie, Yutaka; Tada, Hirokazu: Aso, Yoshio et al. Improving Intramolecular Hopping Charge Transport via Periodical Segmentation of π-Conjugation in a Molecule J. Am. Chem. Soc. 143 2021; 599-603. doi: 10.1021/jacs.0c1056
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