IX-C Development of Multi-Function Integrated Macromolecules and Their Organization on Substrate Surfaces for Planar Molecular-Scale Electronics Circuits

The concept of molecular-scale electronics is now realized for individual components such as wire, diode, switch, and memory cell, but the fabrication of complete molecular-scale circuits remains challenging because of the difficulty of connecting molecular modules to one another. Molecular monolithic technology, which integrates the wiring, transistors, and the required passive elements on a single macromolecule, has been proposed as a promising solution to this problem. In this project we have been trying to establish both the architecture of this novel class of macromolecules and the protocols for their purposive organization on metal/semiconductor substrate surfaces.

IX-C-1 Stepwise Synthesis of Molecular Wire with a Double-Tunnel Junction

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We have developed a synthetic protocol for preciselydefined linear macromolecules with a double-tunnel junction as shown in Figure 1. The nature of intramolecular charge transport in a π -conjugated macromolecule with tunnel junctions is of fundamental importance for single electron/hole device applications. In the field of applied physics metal-molecule-metal double junction systems have been intensively studied so far. In contrast, little attention has been paid to an intramolecular tunnel junction system because of the problem of precise fabrication of tunnel junction structures in a macromolecule. Based on our synthetic approach, a series of intramolecular junction systems will be prepared from various types of non-conjugated molecular blocks and the 1–10 nm long π -conjugated molecular blocks that we have already developed.

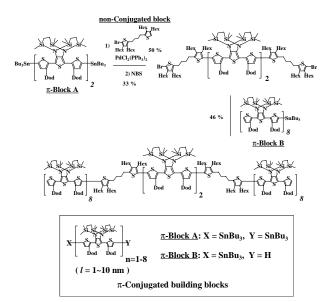


Figure 1. Synthetic scheme of 25 nm long molecular wire with a double-tunnel junction.

IX-C-2 Direct Identification of Conformational Isomers of Adsorbed Oligothiophene on Cu(100)

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A direct conformational analysis using scanning tunneling microscopy (STM) has been performed for individual adsorbed α -octithiophene molecules **8T-Si** on Cu(100). *s-Cis* and *s-trans* conformational isomers are induced by the rotational flexibility of individual thiophene rings. By adding bulky N-silyl substituents to octithiophene, we successfully identify the *s-cis* and *s-trans* conformational isomers using STM. The obtained relative abundances of the *s-cis* and *s-trans* conformations are analyzed using ab initio molecular orbital calculations.