Multifunction Integrated Macromolecules for Molecular-Scale Electronics

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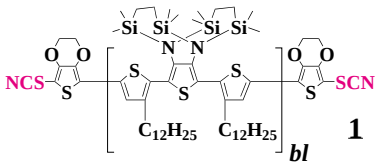
To date there have been demonstrations of molecular-scale diode, switches, transistors, logic circuits, and memory cells, however, the fabrication of complete molecular-scale electronic circuits remains challenging because of the difficulty of connecting molecular device elements to one another. To overcome this problem, we have been developing step-wise synthetic protocols for integrating the molecular functional units required for advanced information processing within a single macromolecule. Our strategy is based on modular architecture using a library of versatile molecular building blocks. The flexible functionality of these blocks is derived from the 3,4-diaminothiophene component, which can be easily modified to tune the structural and electronic properties of the main π-conjugated chain.

1. Thiophene Oligomers for Single-Molecule Charge-transport Measurements

One of the current issues in molecular-scale electronics is to understand and control the charge transport characteristics of single-molecular wires bonded between metal electrodes. To this end, we have synthesized a series of precisely defined oligothiophenes (**1**) ranging in length from 1 to 30 nanometers. These molecular wires have thiocyanate (**-SCN**) anchors that can lead to spontaneous assembly of the wires on Au-based nano-gap electrode systems without activation agents. The systematic nano-scale charge transport measurements using STM break junctions or planar nano-gap electrode systems are now in progress.



***bl* = 1, 2, 3, 4, 5, 6, 7, 8, 10,16, 24**
(*l* = 1 ~ 30 nm)

Figure 1. Structures of oligomers (**1**).

2. Electrical Conductance of Oligothiophene Molecular Wires[1)]

A break junction method using a scanning tunneling microscope has been applied to electrical conductance measurement of newly designed oligothiophene molecules terminated with a thiocyanate group. The tunneling conduction was evident from an exponential decay of the conductance as a function of the molecular length up to ca. 6 nm. The tunneling decay constant was estimated to be 0.1 angstrom^{-1}. The pre-exponential factor was 1.3 × 10^{-6} S, which was smaller than that observed for alkanedithiols.

3. Direct Conformational Analysis of a 10nm Long Oligothiophene Wire[2)]

Conformational variations of a 10 nm long oligothiophene wire (**2**) on Au(111) have been directly visualized by scanning tunneling microscopy (STM). The local bending angles within the wire are well characterized as s-cis/s-trans configurations of individual thiophene rings. We find that the partial stabilization of the metastable s-cis conformation results in the wire bending, which should be influenced by solvent and substituents.

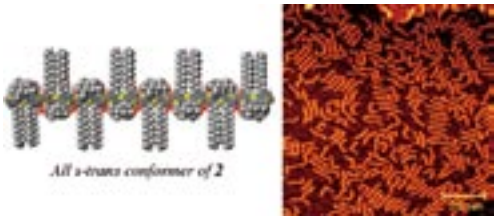


Figure 2. Structure of oligomer (**2**) and Large-area STM image.

References

1) R. Yamada, H. Kumazawa, T. Noutoshi, S. Tanaka and H. Tada, *Nano Lett.* **8**, 1237–1240 (2008).
2) F. Nishiyama, K. Ogawa, S. Tanaka and T. Yokoyama, *J. Phys. Chem. B* **112**, 5272–5275 (2008).