Development of Novel Heterocyclic Compounds and Their Molecular Assemblies for Advanced Materials

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Heterocycles containing sulfur and/or nitrogen atoms are useful as components of functional organic materials since heteroatoms in their rings are helpful to stabilize ions or ion-radical species. In addition, intermolecular interactions caused by heteroatom contacts can be expected to form unique molecular assemblies. In this project, novel functional organic materials based on various heterocycles were synthesized and their physical and structural properties were investigated.

1. (Dibenzoylmethanato)boron Difluoride Derivatives Containing Triphenylamine Moieties: A New Type of Electron-Donor/π-Acceptor System for Dye-Sensitized Solar Cells[1)]

(Dibenzoylmethanato)boron difluoride derivatives containing triphenylamine moieties were synthesized as a new type of electron-donor/π-acceptor system. These new compounds exhibited long-wavelength absorptions in the UV/Vis spectra, and reversible oxidation and reduction waves in cyclic voltammetry experiments. Their amphoteric redox properties are based on their resonance hybrid forms, in which a positive charge is delocalized on the triphenylamine moieties and a negative charge is localized on the boron atoms. Molecular orbital (MO) calculations indicate that their HOMO and LUMO energies vary with the number of phenylene rings connected to the difluoroboron-chelating ring. Dye-sensitized solar cells fabricated by using these compounds as dye sensitizers exhibited solar-to-electric power conversion efficiencies of 2.7–4.4%.

Reference

1) Y. Mizuno, Y. Yisilamu, T. Yamaguchi, M. Tomura, T. Funaki, H. Sugihara and K. Ono, *Chem. –Eur. J.* **20**, 13286–13295 (2014).

Multifunction Integrated Macromolecules for Molecular-Scale Electronics

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Recently a single electron tunnel device (**SET**) has attracted much attention as an ultra-low-power device. In this project, to establish an innovative fabrication process for **SET** systems, we have been developing step-wise synthetic protocols for mono-molecular single-electron tunnel devices and their integrated circuits (**MOSET IC**).

1. Molecular Design for Boosting Conductivity of Deca-Nanometer Scale Molecular Wires

We have already established the synthetic process for "single-nanometer scale" multi-terminal device systems. The next target is to fabricate the "deca-nanometer scale" systems. In this case, one of the fundamental issues is the insufficient conductivity of neutral (undoped) deca-nanometer molecular wires, and so we have been developing the various types of building block for boosting conductivity of long molecular wires by introducing redox-active cites into the conjugated main chain. Figure 1 shows the examples (**1-5**).

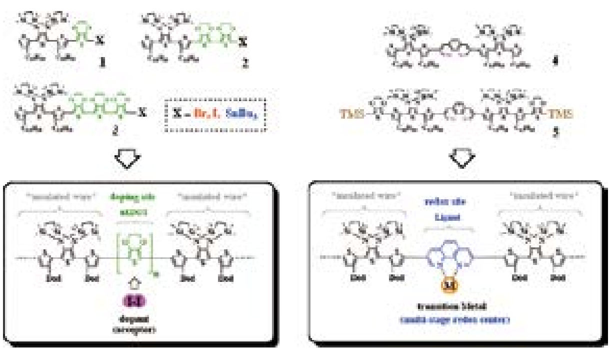

Figure 1. Building blocks for boosting conductivity of long molecular wires.