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

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on various heterocycles were synthesized and their physical and structural properties were investigated.

1. Synthesis, Structure and Physical Properties of *N*-Boc-Pyrrole Derivatives for Organic Semiconductors

attention from the viewpoints of development of organic semiconductor devices.¹⁾ To improve their low solubility, we synthesized several *N-tert*-butoxycarbonyl (Boc)-2,5- diaryl-pyrrole derivatives as precursors of organic semiconductors for the fabrication of solution-processed field-effect transistors. These compounds have nonplanar structures due to a steric hindrance between Boc group and aryl ones. Elimination of Boc group from the soluble precursors by annealing quantitatively afforded insoluble *N*-H-2,5-diarylpyrroles with planar structures. We investigated their spectral and electrochemical changes toward a film fabrication technology.

Reference

 K. Ono, J. Hashizume, H. Yamaguchi, M. Tomura, J. Nishida and Y. Yamashita, *Org. Lett.* 11, 4326–4329 (2009).

Planar π -conjugated molecules have been attracted much

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 (MOSET) and their integrated circuits.

1. Systematic Chemical Modulation of Molecular Wires

We have already elucidated the details of steady-state long-distance molecular conduction through a series of molecular wires **1**. As a next step, we have planed to develop the design principle for precise and wide-range control of electron-transport characteristics of single molecular wires. For this purpose, we have modulated the electronic structure of the wires **1** by systematic chemical modifications. Figure 1 shows the typical examples. The measurement of single molecular conductance of these wires is still in progress.

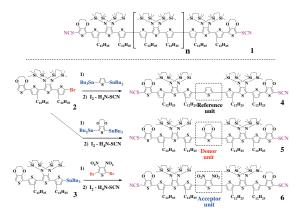


Figure 1. Synthetic scheme for molecular wires with modified electronic structure.