Effects of inserted methylenes on yields and properties of a molecule transistor

MIKU FURUSHIMA[1], MITSUHARU UEMOTO[1], and TOMOYA ONO[1]
Department of Electrical and Electronic Engineering, Graduate School of Engineering, Kobe University, Kobe, Hyogo 657-8501, Japan
furushima@eedept.kobe-u.ac.jp

ABSTRACT

Single molecule transistors are transistors in which a single electron-conductive molecule cross-links a source and drain electrodes as a channel system [1]. It is expected to work due to resonant tunneling effect and realize high-speed operation with low energy-consumption. In this study, we carry out density functional theory (DFT) calculation aiming to realize both high yield of cross-linking structures and high performance as a transistor. The candidate molecules are two kinds of π-conjugated highly fused oligosilole derivatives; one has methylene groups on its edges (figure 1(a)) and the other does not (figure 1(b)).

We first calculate the binding energies of the molecules and Au(111) electrodes to evaluate the yields using conventional plane wave method for DFT calculations. Then, the electronic structures and electron-transport properties of molecules suspended between electrodes are calculated to evaluate the performance of transistors by the real-space scheme for the DFT calculations, which enables us to investigate the electron-transport properties [2].

It is found that the channel molecule with methylene groups is 1.05 eV more stable in binding energy than the molecule without methylene groups. In addition, both the channel molecules exhibit sufficient conductivities derived from resonant tunneling. It is concluded that inserting methylene groups is beneficial because they increase the yield by the rotational degree of freedom, while their insulating property is negligible.

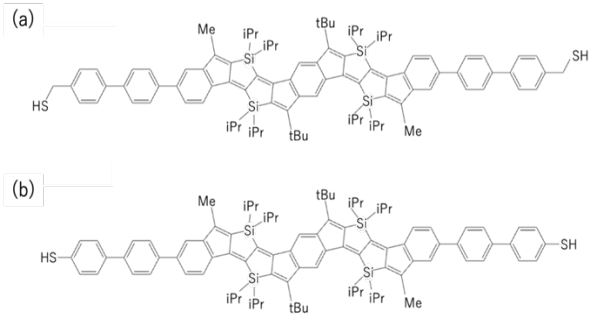

Figure 1: Channel molecule formulas.

References

[1] Lee, S. J.; Kim, J.; Tsuda, T.; Takano, R.; Shintani, R.; Nozaki, K.; Majima, Y. Single-molecule single-electron transistor (SM-SET) based on π-conjugated quinoidal-fused oligosilole and heteroepitaxial spherical Au/Pt nanogap electrodes. *Appl. Phys. Express* **2019**, *12*, 125007.

[2] Ono, T.; Hirose, K. Timesaving Double-Grid Method for Real-Space Electronic-Structure Calculations. *Phys. Rev. Lett.* **1999**, *82*, 5016.