Analysis of Single Molecular Device with Quinoidal Fused Oligosilole Derivatives Based on Scanning Tunneling Microscopy and Scanning Tunneling Spectroscopy

O Seung Joo Lee1, Shuhei Urayama1, Yasuo Azuma1, Ryo Takano2, Ryo Shintani2, Kyoko Nozaki2, and Yutaka Majima1

1 Laboratory for Materials and Structures, Tokyo Institute of Technology, Japan,
2 Graduate School of Engineering, The University of Tokyo, Japan
E-mail: lee@nanoele.msl.titech.ac.jp

π-Conjugated molecules attract a great interest for the application to single molecular devices. In the molecular electronic device, the negative differential resistance (NDR) effect is a very useful function which is characterized by a reduced current with an increase of a voltage bias. With this NDR effect, devices such as molecular switch and memory operation can be proposed. [1] However, π-conjugated molecules often suffer from structural instability for change in their valence charge. Here, we introduce the Si-bridged quinoidal fused oligosilole derivatives, which have an 18 π-conjugated structure with flat a molecular shape (Fig. 1). Because bulky substituents on the Si can effectively suppress molecular interactions, it can be very stable under the air ambient condition. We used the STM (scanning tunneling microscopy) and STS (scanning tunneling spectroscopy) for measuring the tunneling current on the individual molecule based on W-tip/vacuum/molecule/SAM/Au(111) structure at 100 K. Density functional theory calculation gives the molecular orbital information with discrete energy levels, such as HOMO and LUMO levels. [2] It notes that not only the STS results but also the solid-state device results indicate the clear and strong NDR peak at -1.8 V (Fig. 2). This NDR peak should be based on inter-molecular resonance tunneling. For analyzing the mechanism of this molecular device operation, we classified the electrical properties of both the single molecular and inter-molecular structure. Electrostatically, single molecular electrical property was described with double barrier tunneling junction. Moreover, double molecular electrical property was explained by inter-molecular resonance tunneling with NDR. Not only at 100 K, even under the room-temperature condition, this NDR effect was also clearly observed with PVR (Peak to Valley Ratio) of 2 (Fig. 2). While most of molecular devices work at low temperature, this molecular device has strong advantages of room temperature operation. However, it still has many challenges such as reduction of NDR peak voltage and high PVR value.

This study was partially supported by MEXT Elements Strategy Initiative to Form Core Research Center from the Ministry of Education, Culture, Sports, Science, and Technology (MEXT), Japan; and the BK Plus program, Basic Science Research program (NRF-2014R1A6A1030419).


Fig. 1. Molecule structure. Fig. 2. Tunneling current-voltage characteristics: (a) STS (b) Device.