Single-Molecule Charge Transport Properties of Endofullerene

H. Cho[1], S. Fujii[1], M. Kiguchi[1], Y. Hashikawa[2], Y. Murata[2]

[1] *School of Science, Tokyo Institute of Technology, 2−12−1 Ookayama, Meguro-ku, Tokyo 152−8551, Japan*

[2] *Institute for Chemical Research, Kyoto University, Uji, Kyoto 611, Japan*

1614098@ed.tus.ac.jp

Fullerenes and endofullerenes have attracted wide attention due their unique structures, electronic properties, and potential applications in nanoelectronics, nanotechnology, and so on. Endohedral fullerenes containing metal atoms are generally more reactive, either thermally or photochemically, than the corresponding empty fullerenes, because of the small HOMO–LUMO gaps. Electronic properties of individual endohedral fullerenes, thus, remains largely unsolved.

Here, we studied electrical transport characteristics of individual endofullerene using STM-break junction technique [1]. In the break junction technique, metal nano gap is formed between STM tip and substrate. The target molecule diffuse to the nano gap, and bridge the metal electrodes, forming the single-molecule junction. Figure 1 shows conductance histograms of single-molecule junctions of C_{60}, H_2O@ C_{60}, Li^+@ C_{60} constructed from more than 6,000 traces measured at the bias voltage of 100 mV. For each molecule, two prominent peaks [high (H) state and low (L) state] were observed in the histograms. The H and L states were expected to be originated by the single-molecule junctions with different metal-molecule contact configurations. We found that the inclusion of the guest atom or molecule in the C_{60} cage affected the single-molecule conductance of C_{60}. While the inclusion of H_2O caused a small modulation of the single-molecule conductance, the inclusion of Li^+ led to a large increase in conductance by a factor of 2~4. In contrast to the chemically inert H_2O molecule, the active Li^+ ion would strongly interact with the C_{60} cage, which caused the large conductance change.

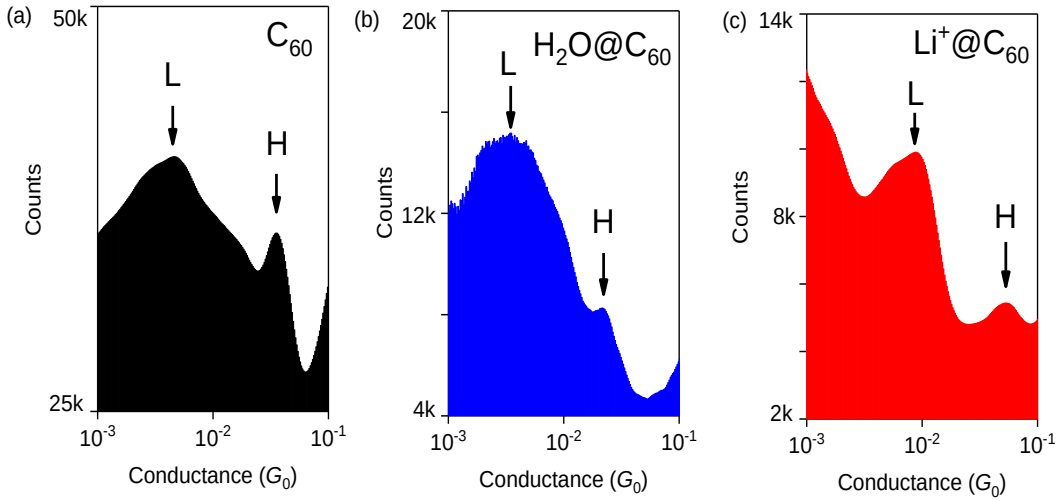

Figure 1: Conductance histograms of single-molecule junction with (a)C_{60}, (b)H_2O@C_{60}, (c)Li^+@C_{60}.

Reference:

[1] M. Koike, S. Fujii, H. Cho, Y. Shoji, T. Nishino, T. Fukushima, M. Kiguchi , *Jpn. J. Appl. Phys*, **57**, 03EG05