C60 フラーレンに閉じ込められた単一水分子の電子誘起分子振動

Electron-induced vibrations of a single water molecule encapsulated in a C60 fullerene

東大生研・ナノ量子機構 [1], 京大化研 [2]
○杜 少卿 [1]、橋川 祥史 [2]、村田 靖次郎 [2]、平川 一彦 [1]
[1]IIS/INQIE, Univ. of Tokyo, [2]ICR, Kyoto University
○Shaoqing Du[1], Yoshifumi Hashikawa[2], Yasujiro Murata[2], Kazuhiko Hirakawa[1]
E-mail: sqdu@iis.u-tokyo.ac.jp

The encapsulation of a single water molecule inside a buckyball [1] provides a unique opportunity to study the dynamics of a single water molecule, since the endofullerene structure can suppress the effect of hydrogen-bond networks by isolating water molecules. However, most of the studies on the $H_2O@C_{60}$ molecules have been performed on a large ensemble of molecules; only a few have been done at the single-molecule level [2].

Here, we have investigated the electron transport through single $H_2O@C_{60}$ molecules by using the single molecule transistor (SMT) geometry [3], as shown in Fig. 1(a). The fullerene works as a natural cage to trap a H_2O molecule [1]. Using the source and drain electrodes separated by a sub-nm gap, we captured a single $H_2O@C_{60}$ molecule in the nanogap electrodes. By performing transport measurement, we have obtained a Coulomb stability diagram of a single-$H_2O@C_{60}$ SMT for the first time. As shown in Fig. 1(b), single electron tunneling area shows six excited states below 25 meV with unequal energy spacings. These tunnel-electron-induced excited states are attributed to the librational motions of the encapsulated H_2O molecule in a C_{60} cage, which is in consistent with DFT calculations and the result of ensemble measurements.

The present result demonstrates that the endofullerene structure together with nanogap electrodes provides a sub-nm-size laboratory for studying single-molecule dynamics.

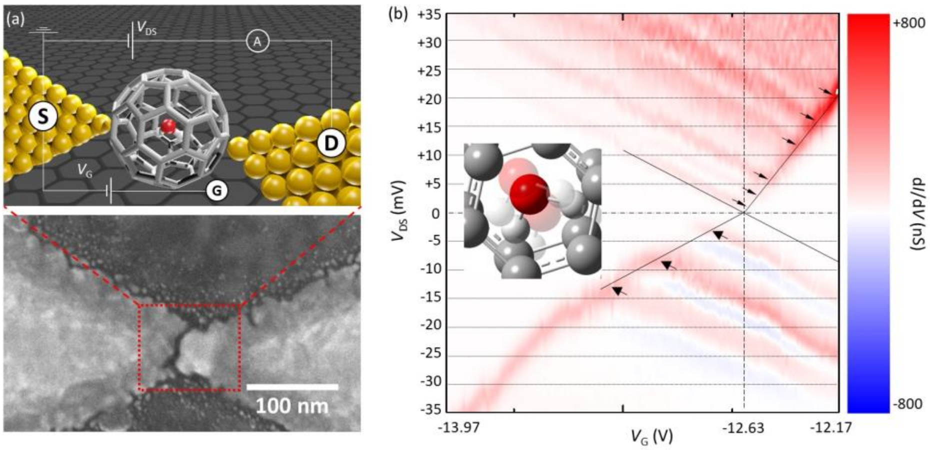

Figure 1 (a) Schematic and SEM image of the nanojunction region of a single molecule transistor (SMT). **(b)** Coulomb stability diagram of a single-$H_2O@C_{60}$ SMT.

Reference:
[1] K. Kurotobi, and Y. Murata, *Science* **333**, 613 (2011). [2] S. Fujii, et al., *Phys. Chem. Chem. Phys.* **21**, 12606 (2019). [3] S. Q. Du, et al., *Nature Photon.* **12**, 608 (2018).