C60 フラーレンに閉じ込められた単一水分子の電荷に依存した分子振動

Charge dependent vibration of a single water molecule encapsulated in a C60 fullerene

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Resolving the charge transport in molecules improves our knowledge on several molecular processes, including chemical reactions, catalysis, and potentially even processes in living organisms. When a molecule is charged, both the electronic structures and vibrational dynamics of the molecule is changed. However, it is very difficult to see such dynamical charge-induced changes.

Here, we have investigated the charge-dependent electron transport through single $H_2O@C_{60}$ molecules [1] by using the single molecule transistor (SMT) geometry [2]. As shown in Fig. 1(a), the very sharp metal electrodes work as THz antennas to tightly confine THz radiation in the gap region [2], and the fullerene works as a natural cage to trap a H_2O molecule. Furthermore, the gate electrode is used to tune the electron number on the molecule, which makes it possible to study charge-induced dynamics of a $H_2O@C_{60}$ SMT. Fig. 1(b) shows the Coulomb stability diagram of a $H_2O@C_{60}$ SMT. The crossing pattern indicates that we capture a single molecule in the nanogap. Then we preformed THz spectroscopy on such $H_2O@C_{60}$ SMT and obtained the charge-dependent spectra of the THz-induced photocurrent, as shown in Fig. 1(c). The peak at 5 meV (dashed line in Fig. 1(c)) appears when an electron is added to the $H_2O@C_{60}$ molecule. The present measurement clearly reveals charge-dependent THz vibration of a single molecule. Also note that the endofullerene structure together with nanogap electrodes can provide a sub-nm-size laboratory for studying single-molecule dynamics.

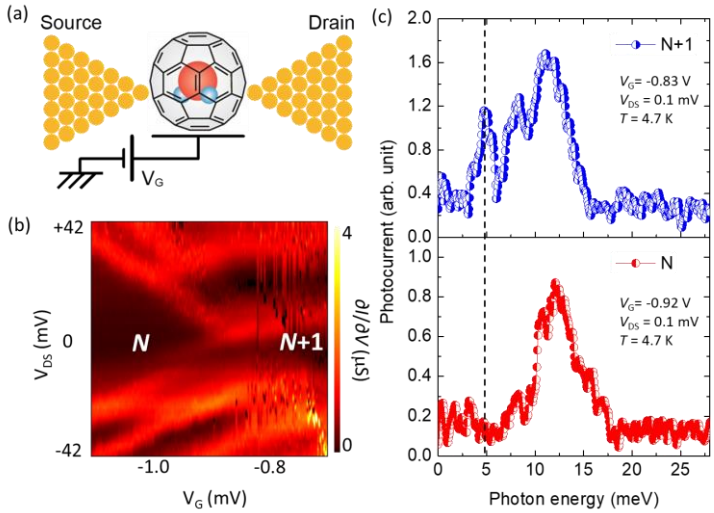

Figure 1 (a) Schematic of a single molecule transistor (SMT). **(b)** Coulomb stability diagram of a single-$H_2O@C_{60}$ SMT. **(c)** Charge dependent spectra of the THz-induced photocurrent in a single-$H_2O@C_{60}$ SMT.

References

[1] K. Kurotobi and Y. Murata, *Science* **333**, 613 (2011).
[2] S. Q. Du, et al., *Nature Photon.* **12**, 608 (2018).