



Transport properties and terahertz dynamics of single molecule transistors

Shaoqing Du,¹ Kenji Yoshida,¹ and Kazuhiko Hirakawa^{1,2}

¹*Institute of Industrial Science, University of Tokyo, Tokyo, Japan*

²*Institute for Quantum Information Electronics, University of Tokyo, Tokyo, Japan*

Terahertz (THz) spectroscopy is a powerful tool for characterizing electronic properties and vibronic excitations in various types of solids, liquids, and gases, and it has been extensively used not only for basic sciences but also for industrial applications. Recently, it has become necessary to understand electronic and vibronic excitations at nanometer (nm)-scale to realize state-of-the-art quantum nanodevices. However, it is extremely challenging to perform THz spectroscopy at nm-scale because the diffraction limit of electromagnetic waves hinders tight focusing of THz radiation.

We have introduced a novel technique for THz spectroscopy that utilizes metal nanogap electrodes [1]. Metal nanogap electrodes integrated with a THz antenna are employed to capture a single molecule. Even extremely weak THz absorption can be detected by measuring the THz-induced photocurrent through the target molecule by employing a single molecule transistor (SMT) geometry. Taking advantage of THz-induced photocurrent spectroscopy, vibrational states [2,3] have been investigated.

Furthermore, we have investigated electron transport through H₂O@C₆₀ SMTs [4] and observed that H₂O@C₆₀ SMTs exhibit three excited states below 10 meV. From comparison between experiment and theory, the excitations observed below 10 meV are identified to be the quantum rotational excitations of the water molecule encapsulated in the C₆₀ cage. Surprisingly, the quantum rotational excitations of both para- and ortho-water molecule are observed simultaneously even when a single water molecule is measured, indicating that the fluctuation between the two nuclear isomer states takes place in a time scale shorter than our measurement time (~1 min), probably due to interaction between the encapsulated water molecule and conducting electrons.

*) present address: Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai, China

[1] K. Yoshida, K. Shibata, and K. Hirakawa, *Phys. Rev. Lett.* **115**, 138302 (2015).

[2] S. Du, K. Yoshida, Y. Zhang, I. Hamada, and K. Hirakawa, *Nature Photon.* **12**, 608 (2018).

[3] S. Du, Y. Zhang, K. Yoshida, and K. Hirakawa, *Appl. Phys. Exp.* **13**, 105002 (2020).

[4] S. Du, Y. Hashikawa, H. Ito, K. Hashimoto, Y. Murata, Y. Hirayama, and K. Hirakawa, *Nano Lett.* **21**, 10346 (2021).