【Grant-in-Aid for Scientific Research (S)】
Broad Section D

Title of Project： **Terahertz dynamics of single molecule transistors and its application to quantum information processing**

HIRAKAWA Kazuhiko
(The University of Tokyo, Institute of Industrial Science, Professor)

Research Project Number: 20H05660　　Researcher Number：10183097
Keyword：single molecule transistors, terahertz radiation, quantum information technology

【Purpose and Background of the Research】

In recent years, single molecules have attracted attention as devices that can apply molecular functions to electronics. Furthermore, molecular vibrations have properties as quantum mechanical oscillators and have a possibility of becoming a new medium for quantum information processing. Since the energies of elementary excitations such as quantum levels and molecular vibrations in such atomic-scale nanostructures corresponds to the photon energy of terahertz (THz) electromagnetic waves, useful information on the physics and dynamics of such quantum nanostructures can be obtained by THz spectroscopy.

Recently, we have formed electrodes with atomic-scale gaps onto a single molecule and used them as THz antennas to focus THz electromagnetic waves on a single molecule. It has become possible to measure extremely weak THz signals derived from excitation within a single molecule.

We think that research on the interaction between THz electromagnetic waves and quantum nanostructures has just entered a new phase. Without missing this timing, we should dig into the physics of the quantum nanostructures and investigate their applications as media for quantum information processing.

The purpose of this research is to further promote and deepen the new field of atomic-scale "terahertz nanoscience" that is currently emerging, and to explore the possibility of its applications.

【Research Methods】

1) Terahertz spectroscopy of single molecules: The molecular vibrations and conduction electrons are strongly coupled and, by coherently controlling the molecular vibrations with THz pulses, we will establish the basis for quantum control of electron conduction and explore the possibility of application to new quantum information processing.
2) Resistive detection of single molecule nuclear magnetic resonance (NMR): We will perform resistive detection of NMR signal of single atoms and molecules by using nanogap electrodes and explore a possibility of using it as a medium for carrying new quantum information.
3) Ultra-strong THz electric fields in the nanogap electrodes: Unprecedented “ultra-strong ac electric fields of ~GV/cm range in the nm region" generated by the field enhancement effect of the nanogap electrodes. We will elucidate novel electron dynamics in such ultrahigh ac fields.
4) Use of nanomechanical structures for advanced nanoscale sensing: We develop a new technology for high sensitivity nanoscale transport measurements and THz spectroscopy using MEMS/NEMS technology.

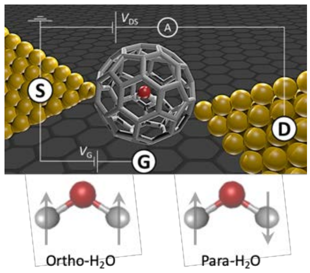

Fig. 1 Schematic illustration of a single molecule transistor structure with a $H_2O@C_{60}$ molecule as a quantum dot.

【Expected Research Achievements and Scientific Significance】

Physics and applications of nm-scale systems are just in a phase of rapid rise and this project will be a major stepping stone. Furthermore, the miniaturization of silicon technology represented by CMOS is approaching its limit, and there is an urgent need to search for new device principles. This research provides a major scientific basis for creating nanodevices with novel functions such as quantum information processing by combining the unique physical properties of nanogap electrodes and molecules.

【Publications Relevant to the Project】

- S. Du, K. Yoshida, Y. Zhang, I. Hamada, and K. Hirakawa: “Terahertz dynamics of electron–vibron coupling in single molecules with tunable electrostatic potential”, Nature Photonics, vol.12, pp. 608-612 (2018).
- K. Yoshida, K. Shibata, and K. Hirakawa: “Terahertz field enhancement and photon-assisted tunneling in single-molecule transistors”, Physical Review Letters, vol. 115, pp. 138302-1~5 (2015).

【Term of Project】 FY2020-2024

【Budget Allocation】 146,800Thousand Yen

【Homepage Address and Other Contact Information】

http://thz.iis.u-tokyo.ac.jp
hirakawa@iis.u-tokyo.ac.jp