【Grant-in-Aid for Transformative Research Areas（Ｂ）】

Establishment of single-molecule electron microscopy and its quantum applications (Single Molecule Quantum)

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Project Information	Project Number : 24B201	Project Period (FY) : 2024-2026
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Purpose and Background of the Research

●Outline of the Research

The project aims to establish the theoretical and experimental methods to fully understand single-molecule electron sources, together with the goal of creating new quantum devices. Single-molecule electron sources are comprised of single-molecule protrusions formed on a metallic needle, as illustrated in Fig. 1(a). These protrusions emit electrons, thus functioning as single-molecule electron sources. By utilizing such electron sources, it is possible to develop an ultrafast switch that surpasses the speed of current computer switches by factors of 1,000 or even 1,000,000. Additionally, leveraging the quantum properties of a single molecule allows for the integration of ultrafast switches into a single molecule without altering its size. Consequently, single-molecule electron sources are anticipated to generate unique quantum devices. However, much remains unknown about these sources. To gain deeper insights, improved numerical models are required, along with detailed observations of their atomic and electronic structures. To achieve these objectives, four interdisciplinary teams have been assembled. As depicted in Figure 1(b), the Kito, Oshima, and Yanagisawa teams will focus on elucidating the underlying physics. Concurrently, the Lambert and Yanagisawa teams will collaborate to explore and develop innovative quantum devices from both experimental and theoretical perspectives.

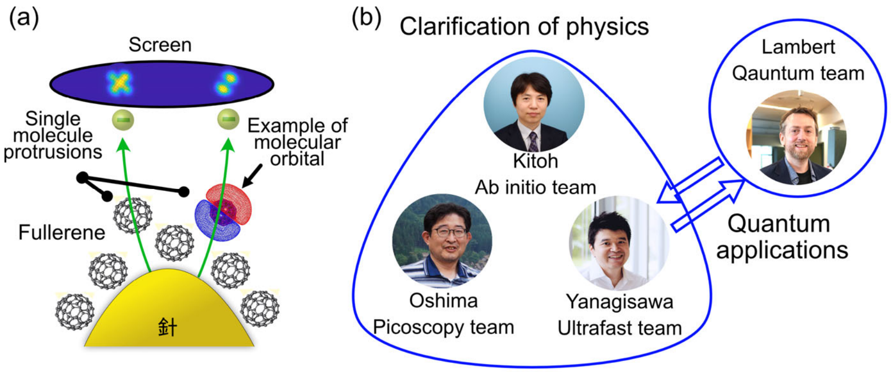

Figure 1. Conceptual diagram of single-molecule electron sources (a) and the team structures (b).

●Single molecular electron sources for high-resolution microscopes

One of the interesting capabilities of single-molecule electron sources is their ability to display the distribution of electrons within a single molecule, known as molecular orbitals (MOs). MOs exhibit distinctive shapes, as illustrated in Figure 1(a). These unique shapes represent one of the quantum properties of electrons. As depicted in Figure 1(a), these MOs can be observed by projecting the distribution of electrons emitted from a single molecule onto a screen.

● Integration of switches

The shape of MOs varies with the electron energies, which is another quantum property of electrons. By changing the energy of the emitted electrons using light, the observed MOs can be altered, for example, from case A to case B in Figure 2. Such phenomena can be observed using the microscope shown in Figure 1(a). This functionality allows for the integration of ultrafast switches into a single molecule without changing its size. Typically, when switches are integrated, the size of the device increases. However, in this scheme, the size remains unchanged. The main focus of this project is to determine how many switches can be integrated using this approach. Additionally, we will develop and explore novel quantum devices based on the quantum properties of single molecules.

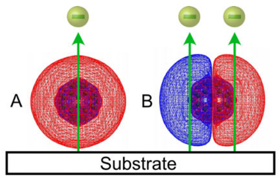

Figure 2. Conceptual diagram of electron emissions from two different molecular orbitals.

Expected Research Achievements

●Project goals

Here, we will develop the following three capabilities: 1. A novel electron microscope capable of revealing the electronic structures of single-molecule electron sources in detail. 2. A method to observe the atomic structures of the electron sources with picoscale precision. 3. A new computational method for predicting the atomic and electronic structures of single-molecule electron sources with high accuracy. With these advancements, our goal is to elucidate the complete details of single-molecule electron sources and develop a method to integrate ultrafast switches into a single molecule, as illustrated conceptually in Figure 3. Additionally, we will clarify the feasibility of creating qubits using this source.

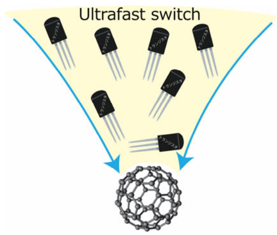

Figure 3. Conceptual diagram of the integration of switches into a single molecule.

●SmoleQ network

Since the keywords of this project are "single molecule" and "quantum", we have named our project Single Molecule Quantum (SmoleQ), affectionately referred to as “Small Q”. Throughout this project, we aim to expand our network and establish connections with leading researchers in various fields. To achieve this, we will invite them to give talks at the SmoleQ seminar and participate in workshops. This initiative will help us build a robust academic community and embark on ambitious projects.

●Outreach activities

The microscopes used in the SmoleQ project can be constructed with a simple setup at a low cost. Typically, expensive equipment costing tens of millions of yen is required to observe MOs. In contrast, the envisioned microscope could be manufactured at a fraction of the cost, ranging from one-hundredth to one-tenth of high-end microscopes. These affordable microscopes could potentially be introduced in schools, allowing students to observe the quantum world, specifically MOs. To achieve this goal, the Quantum Kids Project (QKP) is currently being launched. QKP will work alongside SmoleQ to make the quantum world visible in educational settings.

Homepage Address, etc.	SmoleQ: https://hirofumiyanagisawa3.wixsite.com/smoleq QKP: https://hirofumiyanagisawa3.wixsite.com/quantum-kids-project