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

Exploring molecular science by atomic-scale spectroscopy

Principal Investigator	RIKEN, Cluster for Pioneering Research, Chief Scientist KIM Yousoo	Researcher Number:50373296
Project Information	Project Number : 22H04967 Keywords : Scanning Probe Microscope, Single molecule, Nanospectroscopy	Project Period (FY) : 2022-2026

Purpose and Background of the Research

●Outline of the Research

The structure and properties of matter are closely related to each other. The size of atoms and molecules, the smallest building blocks to make up matter, is in units of nanometers. A nanometer is about 1/100,000th of the thickness of a hair (0.1 mm), and it has been difficult to analyze the structure and measure the physical properties of materials in such a small area. The principal investigator and his colleagues are pioneers in developing a unique nanometrology method that combines scanning tunneling microscopy (STM), a microscope that uses an atomically sharp needle to observe nanoscale structures, and optical technology to detect weak light.

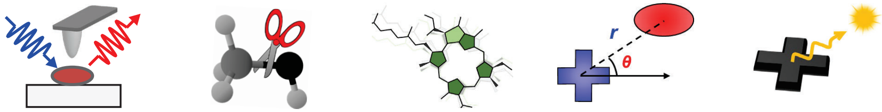
In this project, we will develop our original nanometric method and pioneer a new molecular science by directly linking the nanostructure and physical properties of single molecules (Fig. 1 upper panel). Specifically, we aim to establish more precise measurement techniques (1), expand into various basic research areas (2) to (4), and develop new functions of molecules (5). Through these studies, we will expand the frontiers of materials science and establish basic science in unexplored research areas that will spill over into various fields, including chemical reactions, biology, organic devices, and quantum technology.

In this project

Taking advantage of an extreme nanometrology,

Manipulating structures × Creating new properties

Item (1)	Item (2)	Item (3)	Item (4)	Item (5)
Novel metrology	**Chemical reaction**	**Bio molecules**	**Organic devices**	**Quantum technology**



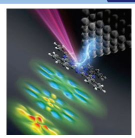
Elucidating fundamental principles for creating new molecular functions
Pioneering new molecular science that will impact diverse fields

So far, we...

Combining STM and Photons

Seeing × Measuring

Establishment of extreme nanometrology



World's leading achievements

Kimura *et al., Nature* 570, 210 (2019).
Jaculbia *et al., Nat. Nano.*15, 105 (2020).
Zhang et al., *JACS* 143, 9461 (2021)
Imada *et al., Science* 373, 95 (2021).
Imai-Imada *et al., Nature* 603, 829 (2022).

Figure 1. An overview of this project

●Establishment of novel measurement technologies & Development of novel molecular science

We will establish a new measurement platform technology by combining atomic force microscope (AFM) capabilities and the nanometrology we have developed to date (Fig.2). AFM is a microscope that detects the tiny force acting between a sharp tip and the object, and can observe individual atomic positions in more detail than STM.

STM, a microscope based on the detection of electric current, can only measure conducting materials. On the other hand, AFM does not require conductivity, and insulators can also be measured.

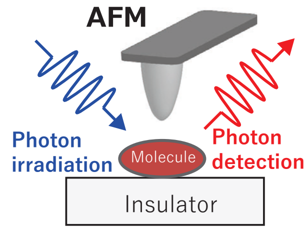


Figure 2. A schematic drawing of novel metrology combining AFM and photon technology

Thus, AFM-based nanometrology are expected to be an important tool for pioneering new molecular science by expanding expand the scope of measurable objects.

Expected Research Achievements

●Establishment of new chemical reaction control methods

A molecule consists of chemical bonds (Fig.3), and the goal of making and breaking these bonds one by one is an important goal for chemists. In this project, we will establish a new reaction control method by making use of AFM technology that can visualize the chemical bonds in a molecule and optical technology that we have been working on.

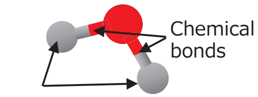


Figure 3. A water (H_2O) molecule and chemical bonds

●Application to biomolecules

We establish new sample preparation methods to measure more various molecules, including biomolecules. Biomolecules have a flexible molecular skeleton as shown in Fig. 4. By linking this structural flexibility with molecular properties, we will develop a new basis for biomolecular science.

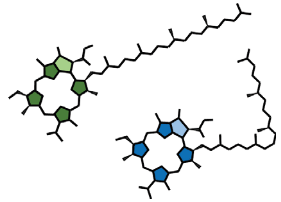


Figure 4. Biomolecules having flexible skeleton structures.

●Construction of scientific basis for organic devices

In organic devices, such as organic light-emitting diodes and organic solar cells, molecules are in close proximity at the nanoscale, and the interactions between the molecules are critical in determining device performance. This project focuses on the molecular arrangement and aims to establish basic science in model experimental systems for organic devices by investigating the relationship between molecular arrangement and physical properties (Fig. 5).

●Establishment of novel molecular quantum technology

Quantum theory views light as particles called *photons*.
A *single-photon source*, which can generate these photons one at a time, is important for future quantum communications.
In this project, we aim to give molecules the ability to act as a new single-photon source by using light to instantly control their structure.

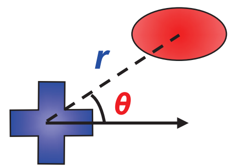


Figure 5. Molecular arrangement

Lab Homepage	http://www2.riken.jp/Kimlab/