【Grant-in-Aid for Scientific Research(S)】
Science and Engineering (Chemistry)

Title of Project：Single Molecule Spectroscopy using Probe Microscope

Maki Kawai
(The University of Tokyo, Graduate School of Frontier Sciences, Professor)

Research Area：Physical chemistry

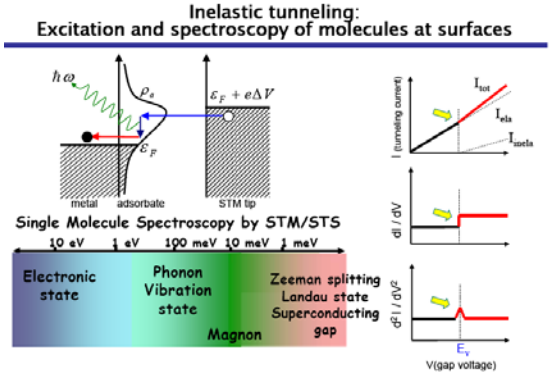
Keyword：Surface/Interface, Single molecule manipulation, Nanoprobes, Molecular spectroscopy

【Purpose and Background of the Research】

Scanning tunneling microscope (STM) is a tool to observe surface structure with very high spatial resolution of sub angstrom. In addition, by investigating elastic/inelastic electron tunneling processes (STS/IETS) through a single molecule, we can acquire electronic and vibrational spectra of each molecule. In this research, we maximize the potential capabilities of STM as a powerful tool for single molecule spectroscopy, explore the exotic behavior of admoleucles and build up fundamental disciplines in the field of moleculer science.

【Research Methods】

In this research, we explore the possibilities of single molecule spectroscopy based on the inelastic tunneling processes as follows:
(1) Tunneling electrons excite vibrations of an adsorbed molecule and induce reaction events such as hopping and bond breaking. We can get the excitation energies by measuring the relation of the events with the injected electron energy as “action spectrum”, and establish the general way to analyze the spectrum.
(2) We challenge to catch the photons ranging from THz to infrared region that are emitted upon the relaxation of vibrationally-excited molecule.
(3) We investigate electronic fine structure associated with the molecular spin by STM-IETS and make clear about the interactions of molecule and substrate electronic system.
(4) Andreev reflection at a interface between magnetic and superconducting materials allows us to measure spin polarization of magnetic materials. Using this phenomenon, we try to evaluate spin-polarized current through a single magnetic atom, molecule and their clusters by STM with a superconducting tip.



【Expected Research Achievements and Scientific Significance】

Following achievements will be expected:
(1) We unveil underlying mechanisms of molecular actions excited by the tunneling electrons and then establish “action spectroscopy” as new single molecule spectroscopy. (2) We make clear about correlation of molecular spin state with the adsorption states. (3) We build an apparatus to catch the photons emitted upon the energy dissipation processes of vibrationally-excited admolecule. The combination with STM-IETS will open a new revenue to build new single molecule spectroscopy. (4) The spin-polarized current through magnetic nano-materials is measured. This research project that we maximize the potential capability of STM-based single molecule spectroscopy is very unique and a great challenge. The findings pave the ways to a frontier in the field of molecular science.

【Publications Relevant to the Project】

・M. Ohara, Y. Kim, S. Yanagisawa, Y. Morikawa and MakiKawai, “Role of Molecular Orbitals near the Fermi Level in the Excitation of Vibrational Modes of a Single Molecule at a Scanning Tunneling Microscope Junction”, *Phys. Rev. Lett.* **100**, 136104 (2008).
・S. Katano, Y. Kim, M. Hori, M. Trenary and M. Kawai, “Reversible Control of Hydrogenation of a Single Molecule”, *Scienc* **316**, 1883 (2007).

【Term of Project】 FY2009-2013

【Budget Allocation】 156,600 Thousand Yen

【Homepage Address and Other Contact Information】

http:// www.surfchem.k.u-tokyo.ac.jp/