



**Title of Project : Studying the Function of Soft Molecular Systems
by the Concerted Use of Theory and Experiment**

Tahei Tahara
(RIKEN, Molecular Spectroscopy Laboratory, Chief Scientist)

【Purpose of the Research Project】

At the frontier of chemical science today is the elucidation and creation of functional, complex molecular systems. They have many degrees of freedom and show enhanced performance, due to their ability to flexibly change their structures. We call such systems “soft molecular systems” and study them by combining molecular science, biophysics, organic and inorganic synthesis, and theory and computation. We investigate biomolecules, supramolecules, molecular assemblies, and soft interfaces by a concerted approach, using theory, advanced spectroscopy, synthesis, and genetic engineering. Through this effort, we create a new innovative research area for the molecular science of complex systems.

【Content of the Research Project】

To study the function of soft molecular systems, we need to examine real systems at the molecular level. It is essential to clarify how a small change in femtoseconds causes a large response in milliseconds – seconds. It is also important to understand how a change in the quantum state of a small part results in the efficient function of a whole system. To achieve this, we carry out research from three different viewpoints, covering large time and space scales:

(1) A01 Group (Theory): This group clarifies the mechanisms behind the efficient functions of soft molecular systems through analysis and prediction based on innovative molecular theories. This group verifies and improves theoretical calculations by comparing them with the experimental data of A02 group, and they design new soft molecular systems with A03 group.

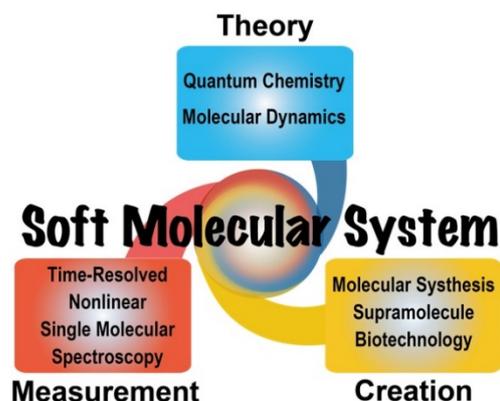
(2) A02 Group (Measurement): This group observes and elucidates metastable states and dynamics of soft molecular systems using cutting-edge advanced experimental methods, such as time-resolved spectroscopy and single molecule spectroscopy. This group clarifies the relationship between the observed dynamical properties and functions, in collaboration with

A01 and A03 groups.

(3) A03 Group (Creation): This group creates new functional, soft molecular systems, using state-of-the-art organic and inorganic synthesis and genetic engineering. With the help of A01 and A02 groups, this group strategically generates new soft molecular systems.

【Expected Research Achievements and Scientific Significance】

The concerted use of theory, measurement, and creation will develop a new research field for predicting, elucidating, and generating new, functional, complex molecular systems. It will provide a basis for new materials science and produce novel tools for related fields such as life science, bioengineering etc.



Concerted use of theory, measurement, and creation to study soft molecular systems

【Key Words】

Molecular system: an assemble of molecules
Biomolecules: molecules that construct a living body, e. g., proteins, nucleic acids, lipids, etc.
Metastable state: a state that is not the most stable but can appear temporally.

【Term of Project】 FY2013-2017

【Budget Allocation】 1,111,000 Thousand Yen

【Homepage Address and Other Contact Information】

<http://www.yawaraka.org/>