

FY2014

JSPS Core-to-Core Program  
-Strategic Research Networks-  
Research Report

Project No.	22003
Research Theme	Photoionisation-induced switch in aromatic molecule-solvent recognition
Duration of Project	April 1, 2012 – March 31, 2015 (36 months)
Core Institution in Japan	Tokyo Institute of Technology

## Implementing Organizations

Country	Japan
Core Institution	Tokyo Institute of Technology
Co-Chair (name and title)	Masaaki FUJII, Professor
Number of Cooperating Institutions	4
Cooperating Institutions	Yokohama City University Tokyo Metropolitan University Kyusyu University Hiroshima University

Country	Germany
Core Institution	TU Berlin
Co-Chair (name and title)	Otto DOPFER, Professor
Number of Cooperating Institutions	2
Cooperating Institutions	University of Düsseldorf, Julius-Maximilians-Universität
Matching Fund	1) Photoionisation-induced switch in aromatic molecule – solvent recognition 2) Electronic structure of protonated aromatic molecules 3) Geometric and electronic structure of silicon-containing aggregates 4) Reactivity and Structure of isolated and solvated flavin ions under cryogenic temperatures in a 22-pole ion trap

Country	England
Core Institution	The University of Manchester
Co-Chair (name and title)	Klaus MÜLLER-DETHLEFS, Professor
Number of Cooperating Institutions	2
Cooperating Institutions	The University of York The University of Oxford
Matching Fund	1) Non-covalent interactions 2) A Novel Instrument for Photodetachment and Photofragmentation Spectroscopy

Country	France
Core Institution	Université Paris Sud
Co-Chair (name and title)	Christophe JOUVET, Professor
Number of Cooperating Institutions	1
Cooperating Institutions	Université d'Aix-Marseille
Matching Fund	1) French National Research Agency (ANR) 2) National Center for Scientific Research (CNRS)

## Result of Program Implementation

This year we have continued the collaborative researches on four following themes.  
(Germany) Structural analysis of ionic cluster studied by EI-IR spectroscopy.  
(UK) Structural analysis of neutral and ionic cluster studied by ZEKE photoelectron spectroscopy.  
(France) Mechanism of molecular switching of protonated ionic cluster studied by electrospray ionization method.  
(Japan) Analysis of photoionization dynamics studied by photoionization-IR spectroscopy.  
We dispatched many young scientists and students in Germany and France intensively and performed the joint experiment to understand the dynamical mechanism of proton-transfer reaction.  
We organized the international symposium "Core-to-Core International Symposium on Ionization Induced Switching" on December 15th (13 oral presentations and 11 poster presentations) in 2014 at TU Berlin that is the cooperating institution in Germany.  
We encouraged young scientists/students to make an English presentation at international conferences such as Gordon Research Conferences: Molecular & Ionic Clusters in Italy and 10th Congress of the World Association of Theoretical and Computational Chemists in Chili etc.

## Achievements in FY2014 (Self Review)

In order to understand the interactions contributed to the higher order structure of biologically relevant molecule such as peptide, protein and DNA, it is very important to understand the aromatic-solvent interactions such as van der Waals forces and vibronic interactions based on hydrogen bonds.  
This year we have investigated the IR spectroscopic and quantum chemical characterization of not only the photoionization-induced molecular switching but also aromatic molecule-solvent hydrogen bond network systems, through the formation of EU-Japan collaborative research network.  
Especially, to understand the photoionization-induced molecular switching, we have demonstrated a new strategy, in which the calculated dynamics are verified by measured time-resolved IR spectra. The coexistence of fast and slow migrations of water molecules around a CONH peptide linkage of trans-acetanilide-water is revealed for a model system representative of a hydrate peptide. This achievement was reported in an *Angew. Chem. Int. Ed. Communication* on page 14601, and announced by *Angew. Chem. Int. Ed. Office* as the work of a German-Japanese collaboration headed by O. Dopfer, M. Fujii, and R. Mitric.  
Clarification of these phenomena is one of the most important targets of these collaborations.

## Future Plan (Measures toward Achieving Research Objectives)

The aromatic molecule-solvent interaction systems are related to the biophysical interactions in the biologically relevant molecules such as peptides, proteins and DNA. The dynamics and energetics of water in biological systems plays a fundamental role in all solvation and biological phenomena in aqueous solution. In particular, the migration of water molecules is the first step that controls the overall process in the time domain.  
This year we demonstrated a new strategy, in which the calculated dynamics are verified by measured time-resolved IR spectra and showed the importance of the fruitful interplay between theory and experiment. But experimentally, the dynamics of individual water molecules is nearly impossible to follow in solution, and there is a lack of experimental data to validate the calculated dynamics.  
In a collaborative effort, a variety of spectroscopic techniques, such as photoionization-IR spectroscopy (Japan), EI-IR spectroscopy (Germany), ZEKE/MATI photoelectron spectroscopy (UK), and electrospray ionization method (France) with theoretical analysis, should be applied to many types of neutral and ionic aromatic molecule-solvent interaction systems to make up for experimental data lack.  
And later, we should concentrate on the more complex species, with the selection strongly depending on the success of generating the species, and the feedback from theoretical analysis and the experimental results of the other groups.