

JSPS Core-to-Core Program
FY2014 Implementation Plan (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 (Co-Chair) Tokyo Institute of Technology
(Masaaki Fujii)

Implementing Organizations

○ **Japan**

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

○ **Partner Countries**

Germany	Core Institution	TU Berlin	
	Co-Chair (name and title)	Otto Dopfer, Professor	
	Cooperating Institutions	University of Düsseldorf	Number of Cooperating Institutions 1

UK	Core Institution	The University of Manchester	
	Co-Chair (name and title)	Klaus Müller-Dethlefs, Professor	
	Cooperating Institutions	The University of York The University of Oxford	Number of Cooperating Institutions 2

France	Core Institution	Université Paris Sud	
	Co-Chair (name and title)	Christophe Juvet, Professor	
	Cooperating Institutions	Université d'Aix-Marseille	Number of Cooperating Institutions 1

Objectives of Research Exchange (including the five years after the project finishes)

The intermolecular interaction in aromatic cationic cluster is rather different from that in the corresponding neutral complex, because of the substantial additional electrostatic, inductive, and charge-transfer attraction arising from the positive charge distribution. Neutral and cationic clusters often have different equilibrium structures and binding energies, corresponding to an ionization-induced switch in the preferred aromatic molecule-solvent recognition motif. These aromatic interactions are closely related to the chemical and biological recognition. This project aims to understand the IR spectroscopic and quantum chemical characterization of aromatic ion-ligand complexes isolated in the gas phase, through the formation of worldwide research network based on the EU-Japan collaboration.

Results to the present

In order to understand the interactions contributed to the higher order structure of biologically relevant molecule such as peptide, protein and DNA, we have investigated the influence of excess energy in the D_0 state on the dynamics of ionization-induced switching systems such as phenol- Ar_n , trans-acetanilide- $(H_2O)_1$, 4-aminobenzonitrile- $(H_2O)_1$, tryptamine- $(H_2O)_1$ etc. Especially, the MATI-IR spectrum of phenol- Ar (1:1) cluster, that is measured by a new IR spectroscopic technique, clearly showed only the free OH stretching vibration at the IE_0 level and thus definitely proved that the π -bound cation of phenol- Ar (1:1) cluster in the vibration-less level did not isomerize to the H-bound cation. Clarification of this phenomenon is one of the next important targets in this project.

Summary of FY 2014 Exchange Plan

Joint Research

We will continue the collaborative research on the 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/MATI 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.

Collaborators including the overseas core institutions will go back and forth in each other's countries to carry out joint experiments. Co-chair (Masaaki Fujii) will visit France in May, UK in November, and Germany in December for the discussion of the collaborative research.

Seminar

We will organize the International symposium for "Photoionisation-induced switch in aromatic molecule-solvent recognition" in December at TU Berlin (Germany). In the symposiums, many Japanese young scientists will have oral and poster presentations of the latest advances in aromatic interactions including photoionisation-induced switching.

Researcher Exchanges

We would like to encourage young scientists / students to make English presentations at the international conferences as follows; The Gordon Research Conferences on Molecular & Ionic Clusters (MIC2014) in Italy, The International Conference on Isolated Biomolecules and Biomolecular Interactions (IBBI 2014) in France (as a part of a joint research in France), The 248th ACS National Meeting in USA, and The 10th Congress of the World Association of Theoretical and Computational Chemists (WATOC 2014) in Chile.