

**JSPS Core-to-Core Program**  
**FY2013 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

UK	Core Institution	Université Paris Sud	
	Co-Chair (name and title)	Christophe Jovet, 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. Hence, neutral and cationic complexes often have rather 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 at 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

We investigated the influence of excess energy in the  $D_0$  state on the dynamics of the mentioned water migration of trans-acetanilide- $H_2O$  (1:1) cation by applying time-resolved ps-UV-UV-IR spectroscopy. As a conclusion, the reducing of the excess energy causes a slowing down of the photoionization induced water migration from the  $CO^-$  to the  $NH^-$  binding site of the trans-acetanilide, but the time-resolved measurements of the IR spectra show that there is no significant change in the reaction pathway. The existence of an intermediate state during the migration has been confirmed. We also found new photoionization induced water migration systems of 4-aminobenzonitrile- $(H_2O)_1$ , tryptamine- $(H_2O)$  etc. These results clearly show the generality of the photoionization induced water migration around peptides.

## Summary of FY 2013 Exchange Plan

### **Joint Research**

We will continue the collaborative research 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/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 and carry out joint experiments.

### **Seminar**

We will organize the International symposium for "Photoionisation-induced switch in aromatic molecule- solvent recognition " in December at The University of Manchester (UK). In the symposiums, many young scientists/students will present the latest advances in aromatic interactions including photoionisation-induced switching by the oral and poster presentation.

### **Researcher Exchanges**

Co-chair (Masaaki Fujii) will visit Germany in July, France in October, and UK in November for the discussion of the collaborative research.

We would like to encourage young scientists/students to make an English presentation at international conferences as follows; Joint symposium between KB-CSJ and BB-KCS in 2013, The 68th meeting: International Symposium on Molecular Spectroscopy, The Asian Chemical Congress, Gordon Research Conferences: Biological Molecules in the Gas Phase & in Solution, The VIIIth Congress of the International Society of Theoretical Chemical Physics, 20th International Conference on Horizons in Hydrogen Bond Research.