

JSPS Core-to-Core Program
FY2012 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	Number of Cooperating Institutions 3

○ **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 Jouvét, Professor	
	Cooperating Institutions		Number of Cooperating Institutions 0

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

The switching of a single water around the peptide bond in trans-acetanilide was observed by picosecond time-resolved IR spectroscopy of trans-acetanilide-H₂O (1:1) cluster cation for the first time. In the neutral state of trans-acetanilide-H₂O (1:1) cluster, the H₂O is hydrogen-bonded to the CO site of the peptide bond. Triggered by photoionization, the H₂O is released from this binding site and eventually trapped after a switching time of 5 picoseconds at the NH site of the same peptide bond. Picosecond time-resolved IR spectra reveal that this water switching is not a simple elementary process but involves an intermediate state, in which H₂O is binding neither to the CO nor the NH site. This result is very important as a first step toward the direct measurement of solvent dynamics around proteins.

Summary of FY 2012 Exchange Plan

Joint Research

We will start 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 symposium for "Photoionisation-induced switch in aromatic molecule-solvent recognition for young investigators" on March at Université Paris Sud (France). In the symposiums, many young scientists/students will present the latest advances in aromatic interactions including photoionisation-induced switching.

Researcher Exchanges

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

We will also encourage young scientists/students to make an English presentation at international conferences as follows: The 16th East Asian Workshop on Chemical Dynamics, 67th meeting; International Symposium on Molecular Spectroscopy, the 14th International Congress of Quantum Chemistry, XXIV IUPAC Symposium on Photochemistry, the 17th International Workshop on Quantum Systems in Chemistry and Physics, Gordon Research Conferences: Gaseous Ions: Structures, Energetics & Reactions etc.