

FY2013

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	1
Cooperating Institutions	University of Düsseldorf
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

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Matching Fund	1) Non-covalent interactions 2) A Novel Instrument for Photodetachment and Photofragmentation Spectroscopy
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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.
Many young scientists and students have gone to England, Germany and France, and carried out many joint experiments.
We organized the international symposium "Core-to-Core International Symposium on Ionization Induced Switching" on December 13th (Poster session) and 16th (Oral session) in 2013 at The University of Manchester that is the cooperating institution in England.
We encouraged young scientists/students to make an English presentation at international conferences such as the 68th International Symposium on Molecular Spectroscopy and The 15th Asian Chemical Congress etc.

Achievements in FY2013 (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, we have achieved the development of a new IR spectroscopy, that is MATI-IR spectroscopy, to understand the detailed mechanism of ionization induced isomerization reaction in PhOH-Ar (1:1) cluster. As a result, the MATI-IR spectrum obtained at the IEO level clearly showed only the free OH stretching vibration and thus definitely proves the vibration-less level of the π -bound cation does not isomerize to the H-bound structure.
Clarification of these phenomena is one of the next 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. Because the most of biologically relevant molecules include simple benzene derivatives (such as phenol, catechol, and tyramine), and the ligands involve rare-gas atoms and water molecules, which represent nonpolar (hydrophobic) and polar (hydrophilic) solvent molecules.
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, shall be applied to many types of neutral and ionic aromatic molecule-solvent interaction systems.
However, for example, photoionization-IR experiments in Japan are quite challenging and cannot be carried out for all biologically relevant molecules. Therefore, the initial focus will be on the simple systems. 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.