

**Priority Area:**

**1. Molecular Structure, Dynamics, and Molecular  
Materials, including Supramolecular Science**

**Coordinators:**

(Japanese)

Keitaro Yoshihara

Vice President

School of Materials Science

Japan Advanced Institute of

Science and Technology,

Hokuriku

(Indian)

C.N.R. Rao

President

Jawaharlal Nehru Centre for Advanced

Scientific Research

**India-Japan Cooperative Science Programme**  
**Activity Report in the Area: Molecular Structure, Dynamics, and Molecular Materials,**  
**including Supramolecular Science**

**Overview and Future Plan**

**1. FY2001-2002 Overview**

Project No. 1

Title: Unconventional magnetic and transport properties in disordered pi system including graphite

T. Enoki

S. V. Subramanyan

TIT

Indian Inst of Sci., Bangalore

Project No. 2

Title: Excited-state structure and relaxation pathway in EDA molecules by time-resolved infrared/Raman spectroscopic measurements

H. Hamaguchi

A. Samanta

Univ. of Tokyo

Univ. of Hyderabad

Project No. 3

Title: Dynamical Behavior of Molecules Confined in a Reverse Micelles

K. Tominaga

K. Bhattacharyya

Molecular Photoscience

Dept. of Phys. Chem.

Research Center, Kobe University

Indian Association for the Cultivation of Science

Seminar No.1

Title: Japan-India Meeting on Molecular and Spramolecular Materials from Chemistry, Physics and Materials Science Aaspects

Toshiaki Enoki

C. N. R. Rao

Tokyo Inst. of Tech.

Jawaharlal Nehru Centre for Adv.

Sci. Res.

Period: March 14-16

Place: Tokyo

Seminar No.2

Title: Structure and Dynamics of Complex Molecular Systems: From a Molecule to a Living Cell

H. Hamaguchi

B. Bagchi

Univ. of Tokyo

Indian Inst.of Sci., Bangalore

Period: 28-29 January, 2003

Place: Tokyo, Japan

**3. Visiting Scientists for Information Exchange**

Visiting Scientist 1

Title: Quantum dynamics of micro-magnetic particles

Dr. S. Ramasesha, Solid State and Structural Chemistry Unit, Indian Inst. of Sci.,

Bangalore visited for 8 days Prof. S. Miyashita, Faculty of Eng., Univ. of Tokyo and exchanged information and made future research plans.

### Visiting Scientist 2

Title: Synthesis and characterization of stable mesoporous materials using triblock copolymer

Dr. G. Raj, Indian Inst. of Sci., Bangalore, visited for 49 days Prof. T. Ohkubo of Faculty of Eng., Univ. of Tokyo and did some preliminary research. He gave a seminar in Univ. of Tokyo and visited several universities.

### Visiting Scientist 3

Title: Electronic and Nonlinear Optical Properties of Organic Thin Films

Prof. T. P. Radhakrishnan, School of Chem., Univ. of Hyderabad visited Prof. T. Nakamura, Inst. of Electronics Sci., Hokkaido Univ. for 15 days and did some preliminary experiments on the above subject.

### Visiting Scientist 4

Title: Ultrafast Electron Transfer Dynamics Using Time-Resolved Infrared Absorption Spectroscopy

Dr. D. Palit, Chem. Div., Bhabha Atomic Research Centre visited for 40 days Prof. K. Yoshihara, Japan Adv. Inst. Sci. and Tech. and did experiment on femtosecond IR study of intermolecular electron transfer.

### Visiting Scientist 5

Title: Development of Properties of Nano-graphite and organic magnetic materials.

Prof. T. Enoki visited Dr. J. V. Yakhmi, BARC, Dr. M. Sastry, Natl. Chem. Inst., Puna, and Prof. C. N. R. Rao, J. Nehru Centre, and Prof. S. V. Subramanyam, IIS and exchange information as well as made a plan for the forthcoming seminar.

## **2. FY2003-2004 Future Plan**

### Project No. 1 (continued)

Title: Dynamical Behavior of Molecules Confined in a Reverse Micelles

K. Tominaga	K. Bhattacharyya
Prof.	Prof.
Kobe Univ.	IACS

(For FY2003, Prof. Bhattacharyya will send his student to perform experiment. Prof. Tominaga may visit Kolkata for a week.)

### Project No. 2

Title: Femtosecond NIR spectroscopic studies of exciplexes, excimers, and conducting organic systems

K. Iwata	S. Umapathy
Assoc. Prof.	Prof.
Univ. of Tokyo	Indian Inst. of Sci., Bangalore

(For FY2003, two Indian scientists will make a visit for 3 weeks each and a Japanese scientist visit for 7-10 days)

### Project No. 3

Title: Electronic and Nonlinear Optical Properties of Organic Thin Films

J. Kawamata	T. P. Radhakrishnan
Associate Prof.	Prof.
Yamaguchi Univ.	Univ. of Hyderabad

(For FY 2003, Prof. Radhakrishnan and his student (Mr. M. Sharath Chandra) will make a visit for 8 weeks from mid September at Yamaguchi Univ. and Hokkaido Univ., and either Prof. Kawamata or Prof. Nakamura and a student visit Hyderabad)

#### Project No. 4

Development of Novel Butadiene Based Photoresponsive Liquid Crystals

Dr. N. Tamaoki

Inst. for Materials & Chem. Process

Natl. Inst. of Adv. Res.

(Details of visit plans should be filed)

Dr. S. Das

Regional Research Laboratory

Council of Scientific and Industrial Research (CSIR)

#### Seminar No.1

Title: Molecular and Supramolecular Materials

Seminar Coordinators:

T. Enoki

Professor

Tokyo Inst. of Tech.

C. N. R. Rao

President

Jawaharlal Nehru Centre for Advanced  
Scientific Research

Period: 2004

Place: India

#### Seminar No.2

Title: Molecular Spectroscopy of Condensed Matter

Seminar Coordinator:

Kankan Bhattacharyya

Indian Association for the Cultivation of Science

Period: 2004 or 2005

Place: Kolkata

Visit Plan

#### Visit Plan No. 1

Title: Development of nanoparticles with surfaces chemically modified by self-assembled monolayer

In FY 2003, Prof. B. L. V. Prasad, National Chem. Lab., Pune will visit Prof. T. Enoki, Dept of Chem., Tokyo Inst. Tech. for 2 weeks.

### **3. Summary**

The two priority areas of the research have been promoted as they were in the past, namely

1) Dynamics of electron transfer and related areas

2) Carbon and molecular materials.

Under these sub-area three joint-research projects were performed and two information-exchange seminars were held in each priority area as summarized above.

The three research projects and two seminars all went very well and successful. Details are given in each report. The two information exchange visits and a short research/information exchange visit were fruitful. More scientists wish to join our programme and that makes the whole plan rather busy.

The scientists who joined the programme are very enthusiastic and most of them are successful in producing good scientific results with a well-considered planning. As a result we jointly published many scientific papers in good journals. The list of publications is given in the following pages.

## Scientific Publications

A. L. Verma, H. H. Thanga, and T. Kitagawa

"Excitation wavelength dependence of photoreduction of cytochrome c and its mechanism monitored by resonance Raman spectroscopy"

*Asian J. Spectrosc.* 5, 97-111 (2001)

B. Venkatesh, H. Hori, G. Miyazaki, S. Nagatomo, T. Kitagawa, and H. Morimoto,

"Coordination geometry of Cu-porphyrin in Cu(II)-Fe(II) hybrid hemoglobins studied by Q-band EPR and resonance Raman spectroscopies"

*J. Inorg. Biochem.* 88, 310-215 (2002)

N. C. Maiti, K. Okamoto, T. Nishino, T. Tomita, and T. Kitagawa,

"Resonance Raman studies on xanthine oxidase: Observation of the Mo(VI)-ligand vibrations"

*J. Biol. Inorg. Chem.* 8, 327-333 (2003)

Anunay Samanta, Satyen Saha, Hironori Ishikawa and Hiro-o Hamaguchi

"Excited State Structure of N-(4-cyanophenyl)carbazole by Time-resolved Infrared Absorption Spectroscopy"

*Chem. Lett.* 340-341 (2002)

Hirohiko Sato, Toshiaki Enoki, A. M. Affoune, B. L. V. Prasad,

"Electrophoretic Deposition of Nano-Sized Diamond Particles",

*Langmuir* 17(2); 547-551 (2001).

A. M. Affoune, B. L. V. Prasad, Hirohiko Sato, Toshiaki Enoki, Yutaka Kaburagi, Yoshihiro Hishiyama,

"Experimental Evidence of a Single Nano-Graphene",

*Chem. Phys. Lett.*, 348 (1-2), 17-20 (2001).

B. L. V. Prasad, Hirohiko Sato, Toshiaki Enoki, Yoshihiro Hishiyama, Yutaka Kaburagi, A. M. Rao, Gamini U. Sumanasekera, and P. C. Eklund,

"Intercalated Nanographite: Structures and Electronic Properties",

*Phys. Rev. B* 64(24), 235407-235416 (2001).

T. Enoki, B. L. V. Prasad, K. Takai, and H. Sato,

"Structural and Electronic Properties of  $sp^2/sp^3$  Mixed Nano-Carbon Systems",

*Mol. Cryst. Liq. Cryst.* 386, 145-149 (2002).

S. Suzuki, H. Yamaguchi, T. Ishigaki, R. Sen, H. Kataura, W. Kraetschmer, and Y. Achiba,  
“Time Evolution of Emission by Carbon Nanoparticles generated with a Laser Furnace Technique”,  
*Eur. Phys. J. D*, 16, 369-372 (2001).

R. Sen, S. Suzuki, H. Kataura, and Y. Achiba,  
“Growth of Single-Walled Carbon Nanotubes from the Condensed Phase”,  
*Chem. Phys. Lett.*, 349, 383-388(2001).

S. Suzuki, R. Sen, T. Tamaki, H. Kataura, and Y. Achiba,  
“Single-Walled Carbon Nanotube Formation with Double Laser Vaporization Technique”,  
*Eur. Phys. J. D*, in press (2003).

H. Kataura, Y. Kumazawa, Y. Maniwa, Y. Ohtsuki, R. Sen, S. Suzuki, and Y. Achiba,  
“Diameter Control of Single-Walled Carbon Nanotubes”,  
*Carbon*, 38, 1691-1697 (2000).

H. Shiromaru, T. Nishide, T. Kitamura, F. A. Rajgara, J. H. Sanderson, Y. Achiba and N. Kobayashi,  
“Snapshot of highly charged molecular ions”,  
*The Physics of Electronic and Atomic Collisions, AIP Conference Proceedings 500*, Y. Ichikawa, K. Okuno,  
H. Tanaka, A. Yagishita and M. Matsuzawa Eds. 636-545 (1999).

T. Nishide, F. A. Rajgara, T. Kitamura, H. Shiromaru, Y. Achiba, and N. Kobayashi,  
“Dissociation of Highly Charged CS<sub>2</sub><sup>q+</sup> Formed by Low Energy Collision of HCl”,  
*Phys. Scripta* T92, 415-419 (2001).

F. A. Rajgara, M. Krishnamurthy, D. Mathur, T. Nishide, T. Kitamura, H. Shiromaru, Y. H. Shiromaru, T.  
Nishide, T. Kitamura, F. A. Rajgara, J. H. Sanderson, Y. Achiba and N. Achiba, and N. Kobayashi,  
“Fragmentation dynamics of CS<sub>2</sub><sup>q+</sup>(q=3-10) molecular ions”,  
*Phys. Rev. A*, 64, 032712(10) (2001).

F. A. Rajgara, D. Mathur, T. Nishide, T. Kitamura, H. Shiromaru, Y. Achiba, and N. Kobayashi,  
“Multi-hit, position-sensitive, time-of-flight spectrometry using MBWC anode”,  
*Int. J. Mass Spectrom. and Ion Phys.* 215, 151-162 (2002).

Masahiko Ichihashi, Tetsu Hanmura, Ramkuber T. Yadav, and Tamotsu Kondow,  
“Adsorption and Reaction of Methanol Molecule on Nickel Cluster Ions, Ni<sub>n</sub><sup>+</sup> (n = 3-11),  
*J. Phys. Chem. A*, 104, 11885-11890 (2000).

Akira Terasaki, Akira Matsushita, Kensuke Tono, Ramkuber T. Yadav, Tina M. Briere, and Tamotsu  
Kondow,

“Electronic States of the Manganese Dimer Ion Probed by Photodissociation Spectroscopy”,  
*J. Chem. Phys.*, 114, 9367-9370 (2001).

Masahiko Ichihashi, Ramkuber T. Yadav, and Tamotsu Kondow,  
“Adsorption of Metal Molecules on Nickel Cluster Ions”,  
Springer Series in Cluster Physics, *Clusters and Nanomaterials*, Eds.: Yoshiyuki Kawazoe, Kaoru Ohno,  
and Tamotsu Kondow, 99-108 (2001).

Akira Terasaki, Akira Matsushita, Ramkuber T. Yadav, Tina B. Briere, Shinichiou Minemoto, and Tamotsu  
Kondow,  
“Electronic and Geometric Structures of 3d Transition-Metal-Cluster Ions”,  
*4<sup>th</sup> Workshop Conference of the Cluster Science and Technology*, 71-74(2000).

Ramkuber T. Yadav, Tetsu Hanmura, Masahiko Ichihashi, Tamotsu Kondow,  
“Adsorption and Reactions of Ni<sub>n</sub><sup>+</sup> Clusters with Methanol Molecule. Internal and Collision Energy  
Perspectives”,  
*Clusters Nanostruct. Interfaces*, 529-534 (2000).

Masahiko Ichihashi, Tetsu Hanmura, R. T. Yadav, and Tamotsu Kondow,  
“Size-Specific Reactions of Nickel Cluster Ions with Simple Molecules”,  
*Phys. Chem. Clusters, Proc. Nobel Symp., 117th*, 315-316 (2001).

Masahiko Ichihashi, Tetsu Hanmura, R. T. Yadav, and Tamotsu Kondow,  
“Size-Specific Reactions of Transition Metal Clusters in Collision with Simple Molecules”,  
*AIP Conf. Proc.*, 576, 975-978 (2001).

### **Modes of Cooperation:**

1. Joint Research Projects
2. Seminars
3. Visiting Scientists for Information Exchange

### **Report**

#### **1. Joint Research Projects**

FY2001-2002

##### **Project No.1**

**Title:** Molecular Structure, Dynamics, and Molecular Materials, including Supramolecular Science

**Objectives:**

**Project Coordinators:**

(Japanese)	(Indian)
Keitaro Yoshihara	C.N.R. Rao
Vice President	President
School of Materials Science	Jawaharlal Nehru Centre for Advanced
Japan Advanced Institute of Science	Scientific Research
and Technology, Hokuriku	

**Date of Commencement:** 1 April 1997

**Date of Completion:** 31 March 2003

**Accomplishment Status:****Future Plan:****Exchange Visits Undertaken**

FY2001

Japan to India

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Hiro-o Hamaguchi Professor University of Tokyo	Excited state structure and relaxation pathway in EDA molecules by time-resolved infrared/Raman spectroscopic measurements	Anunay Samanta, Reader University of Hyderabad	4 Aug.2001- 8 Aug.2001 (5 days)

India to Japan

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Anunay Samanta, Reader University of Hyderabad	Excited state structure and relaxation pathway in EDA molecules by time-resolved infrared/Raman spectroscopic measurements	Hiro-o Hamaguchi Professor University of Tokyo	2 Jun..2001- 25 Jul..2001 (54 days)
Vishnubhotla Prasad Dr. Indian Institute of Science	amorphous carbon films and high temperature superconductors	Toshiaki Enoki Professor Tokyo Institute of Technology	16 Jan.2002- 15 Feb.2002 (31 days)
Dipak Kumar Palit Doctor Bhabah Atomic Research Centre	Influence of Hydrogen Bond Dynamics on the Electron Transfer and Subsequent Solvaton Processes in the Excited State of Caumarin 102-Aniline Hdrogen Bonded Complex	Keitaro Yoshihara Vice President Japan Advanced Institute of Science and Technology, Hokuriku	3 Feb.2002- 29 Mar.2002 (55 days)

## FY2002

### Japan to India

Name and Affiliation	Research Subject	Main Host	Period
Toshiaki Enoki Professor Tokyo Institute of Technology	Electronic and Magnetic Properties of Nano-Graphic, Disordered Carbons, and Organic Charge Transfer Complex-Based Molecular Magnets	V.Subramanyan Professor Indian Institute of Science, Bangalore	6 Mar.2003- 13Mar.2003 (8 days)

### India to Japan

Name and Affiliation	Research Subject	Main Host	Period
Govinda Raj Doctor, Indian Institute of Science, Bangalore	Synhtesis of Zeolite Materials and Their Application to the Catalytic Reactors	Tatsuya Ohkubo Professor University of Tokyo	21 Oct..2002- 6 Dec..2002 (47 days)
Anunay Samanta, Reader University of Hyderabad	Structure and Dynamics of EDA Complexes by Time-Resolved Infrared and Raman Spectroscopy	Hiro-o Hamaguchi Professor University of Tokyo	9 May.2002- 30 May.2002 (22 days)
Indranil Rudra Phd Student Indian Institute of Science, Bangalore	Quantum Dynamics in Nanoscale Molecular Magnets	Seiji Miyashita Professor University of Tokyo	20 Jul.2002- 31 Aug.2002 (43 days)
T.P.Radhakrishnan Associate Professor, University of Hyderabad	Electronic and Nonlinear Optical Properties of Organic Thin Films	Takayoshi Nakamura Professor Hokkaido University	20 Nov.2002- 4 Dec.2002 (15 days)

## Project No. 2

**Title:** Dynamical Behavior of Molecules Confined in a Reverse Micelles

### **Objectives:**

Reactive environments are known to favorably facilitate many chemical and physical processes. The efficiency of biological reactions is attributed, in part, to the highly structured environments. Catalytic processes are enhanced by employing gels, micelles, polymers, zeolites, and biological membranes. To investigate the effects of structured environments on chemical dynamics, it is advantageous to choose simple models with well-characterized physical and chemical attributes. Micellar solutions are model systems that have been used extensively to investigate restricted environments. Reverse micelles are composed of a polar solvent restricted by a surfactant in a nonpolar solvent, forming a well-defined solvent pool. These isolated solvent pools can be thought as a nano-reaction field. Reactivity is often enhanced by the micellar structure and size, and unique nano-environment. In this collaboration research program Bhattacharyya and Tominaga will combine characteristic features of the two researchers; knowledge and experience of Bhattacharyya on the studies of reverse micelles and experimental and theoretical techniques

of Tominaga on the femtosecond laser spectroscopy. The combination of the two features will bring new aspects on the dynamical studies of reverse micelles.

**Project Coordinators:**

(Japanese)	(Indian)
Keisuke Tominaga	Kankan Bhattacharyya
Professor	Professor
Molecular Photoscience	Department of Physical Chemistry
Research Center	Indian Association for the Cultivation of Science

**Date of Commencement:** 1 January 2002

**Date of Completion:** 31 March 2004

**Accomplishment Status:**

The project has started by mutual visit between Tominaga and Bhattacharyya. During the period from January 23 to Feb. 2, 2002, Bhattacharyya visited Japan and learnt several new techniques at the Tominaga's laboratory, planned many possible experiments, gave an invited talk at the Second Asian Conference on Ultrafast Phenomena, and visited Tokyo and Kyoto. During the stay in Kolkata from December 14 to 19, 2002, Tominaga gave three lectures on his recent research about dynamics in liquids. Bhattacharyya and Tominaga discussed possible experiments by the ultrafast laser applied to dynamics in soft confined systems such as lipids and reverse micelles. They finalized several possible experiments, and it was decided that one student of Bhattacharyya may visit Kobe for a certain period and do ultrafast experiments on these systems. Tominaga and Bhattacharyya were invited to give a talk in the Indo-Japan Seminar on January 28, 29, 2003 in Tokyo. They discussed their recent progress of the experiments on dynamics in micelles.

Bhattacharyya has discovered that the solvation time of a water pool in reverse micelles is more than four orders of magnitudes smaller than that of bulk water. This is a striking discovery which stimulates many theoreticians on liquid dynamics as well as experimentalists of ultrafast laser field. The next questions to be asked are how the probe molecules exist in the water pool and how the solvation time depends on the microscopic state of the probe in the micelles. To answer these questions Bhattacharyya and Tominaga have started static and dynamic measurements on the probe molecules confined in the water pool. The preliminary results have been already obtained.

**Future Plan:**

Bhattacharyya and Tominaga will continue the planned experiments of static and dynamic spectroscopy on the probe in a water pool of the reverse micelles. Bhattacharyya will send his student to Tominaga for a certain period to do ultrafast laser experiments. The experiments they planned for the dynamic on the micelles are optical nonlinear spectroscopy in the infrared region and time-correlated single photon counting. Tominaga may visit Kolkata to summarize the project in the end of the fiscal year.

## Exchange Visits Undertaken

FY2001

India to Japan

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Kankan Bhattacharyya Professor, Indian Association for the Cultivation of Science	Dynamical Behavior of Molecules Confined in a Reverse Micelles	Keisuke Tominaga Professor Kobe University	23 Jan. 2002- 2 Feb. 2002 (11 days)

FY2002

Japan to India

<u>Name and Affiliation</u>	<u>Research Subject</u>	<u>Main Host</u>	<u>Period</u>
Keisuke Tominaga Professor Kobe University	Dynamical Behavior of Molecules Confined in a Reverse Micelles	Kankan Bhattacharyya Professor, Indian Association for the Cultivation of Science	14 Dec. 2002- 20 Dec. 2002 (7 days)

FY2003

### Project No.1

**Title:** Dynamical Behavior of Molecules Confined in a Reverse Micelle

#### Project Coordinators:

(Japanese)	(Indian)
Keisuke Tominaga	Kankan Bhattacharyya
Professor	Professor
Molecular Photoscience Research Center Kobe University	Department of Physical Chemistry Indian Association for the Cultivation of Science

**Date of Commencement:** 1 January 2002

**Date of Completion:** 31 March 2004

#### Research Plan

June, 2003-January 2004: Ultrafast spectroscopic measurements on reverse micelles

(a)excitation wavelength dependence on the fluorescence decay of dyes in water pools of reverse micelles.

Fluorescent probe dyes (coumarin 343, DCM) are dissolved in water pools of reverse micelles such as AOT. Time resolved fluorescence spectra are measured by single photon counting apparatus. The excitation wavelength is tuned from 390 nm to 460nm. The time correlation function of the solvation dynamics is obtained from the time-resolved spectra.

(b)3-pulse photon echo peak shift measurement on the OH stretching of water in the reverse micelles.

3-pulse photon echo peak shift measurement is performed on the OH stretching mode of water of water pools in reversed micelles with infrared short pulses (pulse width ~ 150fs). The measurement is done by changing the size of the micelles.

January 2004: Tominaga will visit Kolkatta for one week to discuss results of the above experiments.

### **List of Members of Research Team**

From Japan

**Keisuke Tominaga**

**Professor, Kobe University**

Kaoru Ohta

Postdoctoral fellow, Kobe University

From India

**Kankan Bhattacharyya**

**Professor, Indian Association for the Cultivation of Science**

### **Project No.2**

**Title:** Femtosecond near-infrared spectroscopic studies on charge carrier dynamics, exciplex dynamics and organic pigments

### **Project Coordinators:**

(Japanese)

(Indian)

Koichi Iwata

Siva Umamathy

Associate Professor

Professor

**The University of Tokyo**

**Indian Institute of Science**

**Date of Commencement:** 1 April 2003

**Date of Completion:** 31 March 2006

### **Research Plan:**

We prove to undertake studies on photoinduced transients in polymeric systems, quinones – aromatic methylene exciplex and bianthryl derivatives. Photoexcitation would be carried out using both 270nm and 400nm. The transients would be observed in the NIR region (900-1600nm). We hope to observe both time resolved absorption spectra and also time dependence in specific wavelength and time dependent, would be converted into frequency spectrum. These data, life times, oscillation frequencies and corresponding dephasing times, would then be analysed to understand the dynamics associated with the photochemical and photophysical processes. In addition, we propose to carry out many of these experiments in different solvent conditions (of varying dielectric constant) and also binary solvent mixtures. This we hope would provide further understanding of the solvent control of the above processes.

The specific systems to be studied includes, polyaniline, polyvinylcarbazole, flouranil-methoxy, naphthalene exciplex, 10-ethylaminobianthryl, 10-cyanobianthryl, 10-cyano-10'-dimethylaminobianthryl, and 9-anthrylcarbazole.

First Year: Polyaniline and Two bianthryl derivatives

Second Year: Polyvinyl Carbazole and other bianthryl derivatives

Third Year: Quinone exciplexes and other experiments that might need to be repeated and any other experiments required to substantiate the observed results.

### **List of Members of Research Team**

From Japan

**Hiro-o Hamaguchi**                      **Professor, The University of Tokyo**

From India

Siva Umopathy                      Professor, Indian Institute of Science

Anunay Samanta                      Professor, University of Hyderabad

### **Project No.3**

**Title:** Electronic and nonlinear optical properties of organic thin films

#### **Project Coordinators:**

(Japanese)

Jun Kawamata

Associate Professor

Yamaguchi University

(Indian)

Radhakarishnan Thavarool Puthiyedath

Professor

University of Hyderabad

**Date of Commencement:**                      1 April 2003

**Date of Completion:**                              31 March 2005

#### **Research Plan**

1. Mr. M. Sharath Chandra will visit Yamaguchi University from Nov. 1 for 3 weeks. He will study the SHG characteristics of the films. If the film is not stable enough, then efforts will be made to fabricate the improved films by improving upon the observed results. In addition, Mr. M. Sharath Chandra will train students in Kawamata's group in the technique of (LBL) film. The obtained LBL films will be also characterized by SHG measurements.
2. After studies at Yamaguchi, Mr. M Sharath Chandra will move to Hokkaido University for two weeks. He will do atomic force microscope (AFM) and scanning tunneling microscope (STM) measurements so as to reveal microscopic characteristics of the obtained films at Nanotechnology Research Center of Hokkaido University. In addition, the conductivity and microscopic characteristics of the newly developed films composed of conducting polymers and ionic polymers will be studied at Nakamura's laboratory.
3. Kwamata will visit University of Hyderabad with Nakamura. The results of the experiments that Sharath Chandra conducted at Yamaguchi and Hokkaido will be discussed with all the members concerned. Based on the discussion, the subsequent strategy will be decided. After the discussion, Kawamata and Nakamura will join Japan-India seminar which will be held on March 18-19 at Bangalore and will report the interim results.

#### **List of Members of Research Team:**

From Japan

Jun Kawamata                      Associate Professor, Yamaguchi University

Takayoshi Nakamura                      Professor, Hokkaido University

From India

T. P. Radhakrishnan                      Professor, University of Hyderabad

M. Sharath Chandra                      Ph. D. Student, Senior Research Fellow, University of Hyderabad

#### **Project No.4**

**Title:** Development of novel butadiene based photoresponsive liquid crystals

#### **Project Coordinators:**

(Japanese)

Nobuyuki Tamaoki

Group Leader

National Institute of Advanced

Industrial Science and Technology

(Indian)

Suresh Das

Scientist EII & Head

Council of Scientific and Industrial Research

**Date of Commencement:**

1 April 2003

**Date of Completion:**

31 March 2006

#### **Research Plan**

First Year (2003-2004)

a) Synthesis of newly designed butadiene based liquid crystalline molecules, purification and characterization using spectroscopic methods including NMR, FTIR, UV-Vis and analytical methods such as CHN and HRMS.

b) Study of their mesogenic properties using DSC and polarizing optical microscopy

c) Study of the effect of photoisomerization of butadiene chromophore on the pitch length of dicholesteryl esters

Second Year (2004-2005)

a) Study of photochemical and photophysical properties of these molecules in solution using time-resolved and steady-state techniques

b) Study of photochemical processes in liquid crystalline phases of these materials with the aim of inducing photoinduced isothermal phase transition in these materials

c) Synthesis, purification and characterization of butadiene linked cholesteryl derivatives and study of photoeffects in these mesogens.

Third Year (2005-2006)

a) Synthesis and characterization of hydrogen-bonded mesogens containing butadiene chromophores substituted with pyridyl moiety as the hydrogen bond acceptor. Investigation of the binary phase diagram of these materials with suitable hydrogen bond donors.

b) Synthesis of polymeric LCs containing butadiene chromophore and investigation of their photochemical and photophysical properties

#### **List of Members of Research Team:**

From India

Riju Davis

Research Fellow, Ph.D., Council of Scientific and Industrial Research

Shibu Abraham

Research Fellow, Council of Scientific and Industrial Research

From Japan

Haruhisa Akiyama

Researcher, National Institute of Advanced Industrial Science and

Technology

## 2. Seminars

FY2001

### Seminar No.1

**Title:** Japan-India Meeting on Molecular and Supramolecular Materials

**Objectives:**

Information exchange on molecular and supramolecular materials from chemistry, physics and materials science aspects, and discussion on future prospects of Japan-India collaboration.

Seminar Coordinators:

(Japanese)

Toshiaki Enoki

Professor

Tokyo Institute of Technology

(Indian)

C. N. R. Rao

President

Jawaharlal Nehru Centre for Advanced  
Scientific Research

**Period:** 14-16 March, 2002

**Place:** Tokyo, Japan

**Accomplishment Status:**

Discussion was made on various kinds of molecular and supramolecular systems including inorganic open-framework structures, carbon nanotubes, nanographite, fullerenes, self-assembled molecular systems, molecular modulation, nanometer-size thin films, single molecule magnet, photoactive molecular magnets, organic LED materials, electro-optics design of supramolecular structure, photo-induced transport, electron/ion conductors etc. Future collaborations were also discussed in these rapidly progressing area.

### **Program and Participants**

**14 March (Thu)**

19:00 Dinner

**15 March (Fri)**

9:00- 9:10 Opening Address

9:10- 9:45 New Insights into Inorganic Open-Framework Structures

9:45-10:20 Recent Progress in the Work on Carbon Nanotubes

Coffee Break

10:40-11:15 Single Molecule Magnet (Theory)

11:15-11:50 Molecular Magnets with Photo-Functionality

11:50-12:25 Electron-Hole Recombination Dynamics in Organic LED Materials

Lunch

14:20-14:55 Raman Spectroscopy of Single Carbon Nanotube

14:55-15:30 Electronic Properties of Nano-Graphite

Coffee Break

- 15:50-16:25 X-ray Scattering Studies of Nanometer Sized Thin Films and Multilayers  
16:25-17:00 Phase Transition of Self-Assembled Monolayers  
17:00-17:35 Molecular Materials for SHG and Electro-Optics-Design of Optical Supramolecular Structures  
17:35-18:10 Molecular Modulation of Materials Properties Using Surfactant Assemblies  
19:00-21:00 Banquette

**16 March (Sat)**

- 9:00- 9:35 Photo-Induced Transport in Organic Solids  
9:35-10:10 Assembly of Molecular Conductors and Magnets towards Molecular Electronics

Coffee Break

- 10:30-11:05 Assembly of Nanoscale Structures Using Weak Interactions  
11:05-11:40 Self-Assembled Molecular Systems  
11:40-11:50 Closing Address

**List of Participants**

**From Japan:**

Saburo Nagakura	Chairman, Kanagawa Academy of Science and Technology
Keitaro Yoshihara	Vice President, Japan Advanced Institute of Science and Technology, Hokuriku
Toshiaki Enoki	Professor, Faculty of Science, Tokyo Institute of Technology
Sumio Iijima	Professor, Faculty of Science and Technology, Meijo University
Masahiko Hara	Team Leader, Frontier Research System, The Institute of Physical and Chemical Research (RIKEN)
Takayoshi Nakamura	Professor, Research Institute for Electronic Science, Hokkaido University
Makoto Fujita	Professor, School of Engineering, Nagoya University
Seiji Miyashita	Professor, School of Engineering, University of Tokyo
Kazuhito Hashimoto	Professor, Research Center for Advanced Science and Technology, University of Tokyo
Riichiro Saito	Associate Professor, Faculty of Electro-Communication, University of Electro-Communication

**From India:**

C.N.R. Rao	President, Jawaharlal Nehru Centre for Advanced Scientific Research
S.Ramasesha	Professor, Solid State and Structural Chemistry Unit, Indian Institute of Science
S.Bhattacharya	Associate Professor, Department of Organic Chemistry, Indian Institute of Science
K.S.Narayan	Associate Professor, Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research
M.K.Sanyal	Head, Surface Physics Division, Saha Institute of Nuclear Physics

M.Sastry                                      Scientist E-1, Materials Chemistry Division, National Chemical  
Laboratory  
T.P. Radhakrishnan                      Associate Professor, School of Chemistry, University of Hyderabad

FY2002

**Seminar No.2**

**Title:** Structure and Dynamics of Complex Molecular Systems: From a Molecule to a Living Cell

Objectives: To gather selected leading researchers of physical chemistry from the two countries, both senior and junior, and experimentalists and theoreticians, and provides ideal environment and atmosphere for discussing the hot issues on the structure and dynamics of complex molecular systems, from a molecule to a living cell.

Seminar Coordinators:

(Japan)

Hiro-o Hamaguchi

Professor

The University of Tokyo

(India)

Biman Bagchi

Professor

Indian Institute of Science, Bangalore

**Period:** 28-29 January, 2003

**Place:** Tokyo, Japan

**Accomplishment Status:**

An agreement has been reached, based on fruitful academic exchanges accomplished during the symposium, that next meeting will be held in Calcutta in the year 2004 and that the continuous sponsorship of JSPS and DST will be enthusiastically requested.

**Program and Participants**

**List of Participants**

**From Japan:**

Saburo Nagakura

Keitaro Yoshihara

Hiroo Hamaguchi

Iwao Omine

Keisuke Tominaga

Masahide Terajima

Tahei Tahara

Tatsuo Arai

Takashi Ogura

Koichi Iwata

Chairman, Kanagawa Academy of Science and Technology

Vice President, Japan Advanced Institute of Science and Technology,  
Hokuriku

Professor, University of Tokyo

Professor, Institute for Molecular Science, Okazaki National Research  
Institutes

Professor, Kobe University

Professor, Kyoto University

Team Leader, Molecular Spectroscopy Laboratory, The Institute of  
Physical and Chemical Research (RIKEN)

Professor, University of Tsukuba

Associate Professor, University of Tokyo

Associate Professor, University of Tokyo

Satyen Shaha  
S. Watgaonkar

Doctor, University of Tokyo  
Doctor, Tohoku University

**From India:**

B. Bagchi

Professor, Indian Institute of Science, Bangalore

S. Umamathy

Professor, Indian Institute of Science, Bangalore

A. Samanta

Professor, University of Hyderabad

D. Palit

Bhaba Atomic Research Centre

N. Periasamy

Professor, Tata Institute of Fundamental Research

K. Bhattacharyya

Professor, Department of Physical Chemistry, Indian Association for the Cultivation of Science

FY2003

**Seminar No.3**

**Title:** 2<sup>nd</sup> India-Japan Meeting on Molecular and Supramolecular Materials

**Objectives:** The scientific exchange in the field of molecular materials between Japan and India have been growing in last six years, in which personnel exchange and collaboration works have been stimulated. India-Japan Meeting on Carbon Science and Japan-India Meeting on Molecular and Supramolecular Materials were held in Bangalore in 1998 and in Tokyo in 2002. These meetings have stimulated bilateral scientific exchanges, giving offspring in several aspects. The proposed meeting titled "2<sup>nd</sup> India-Japan meeting on molecular and supramolecular materials will be held in Bangalore with the purpose of enhancing bilateral scientific exchange and collaborations in this field on the basis of growing activities in these two countries.

Seminar Coordinators:

(Japan)

Toshiaki Enoki

Professor

Tokyo Institute of Technology

(India)

Chintamani Nagesa Ramachandra Rao

President

Jawaharlal Nehru Center for Advanced Scientific Research

**Period:** 16-21 March, 2004

**Place:** India

**Expected Effects:** The meeting we propose is planned on the basis of the ongoing bilateral collaborations and also for enhancing further scientific exchanges between the two countries. There are several plans of collaboration now. The proposed meeting is expected to contribute to add more stimuli to the bilateral scientific exchanges by involving more groups working actively in the field of molecular and supramolecular materials science.

**Program and Participants**

The Topics involved are nanocarban systems, supramolecular materials, molecular magnets, single-molecular magnets, spintronics, redox conjugated complexes, self-assembled molecular systems, and multifunctional molecular systems. The program scheduled in two days, March 18 and 19, 2004, consists of presentations of six Japanese delegates and eight Indian delegates, who are working as leaders of the field

concerned in both countries. After the meeting, two of the Japanese delegates are planning to visit laboratories related to the subjects concerned for two days.

### **List of Participants**

**From Japan:**

Takayoshi Nakamura	Professor, Hokkaido University
Seiji Miyashita	Professor, The University of Tokyo
Hiroshi Nishihara	Professor, The University of Tokyo
Kunio Agawa	Professor Nagoya University
Kouichi Kusakabe	Associate Professor, Osaka University
Toshiaki Enoki	Professor, Tokyo Institute of Technology

### **3. Visiting Scientists for Information Exchange**

FY2002

India to Japan

Name and Affiliation	Research Subject	Main Host	Period
S.Ramasesha Professor Indian Institute of Science	Quantum Dynamics of Molecular Magnets	Seiji Miyashita Professor University of Tokyo	21 Oct..2002- 6 Dec..2002 (47 days)

Plan for FY2003

Japan to India

Name and Affiliation	Research Subject	Main Host	Period
A. Miyazaki Research Associate Tokyo Institute of Technology		Jatinder Vir Yakhmi	22 Feb.2004- 5 Mar. 2004 (13 days)