Joint Studies Programs

As one of the important functions of an inter-university research institute, IMS facilitates joint studies programs for which funds are available to cover the costs of research expenses as well as the travel and accommodation expenses of individuals. Proposals from domestic scientists are reviewed and selected by an interuniversity committee.

(1) Special Projects

A. The Third Phase of π-Electron-Based Solid State Science

KATO, Reizo (*RIKEN*)
NAKAZAWA, Yasuhiro (*Osaka Univ.*)
OGATA, Masao (*Univ. Tokyo*)
UJI, Shin-ya (*NIMS*)
TERASAKI, Ichiro (*Nagoya Univ.*)
YAMAMOTO, Hiroshi (*IMS*)

Recently, physical properties of molecule-based π-electron systems are attracting much attention not only because of the advancement in organic electronics such as OLED (= organic light-emitting-diode), OFET (= organic field-effect-transistor), and OPV (= organic photovoltaics) but also because of the discovery of advanced functionality such as electronic ferroelectrics, superconducting transistors, electron glass, quantum spin-liquid, and light-induced ultrafast phase transitions. Those new phenomena sometimes requires researchers to reconsider their way of understanding on electronic states in solids, because they seem to be emerging from spatiotemporal inhomogeneity that has not been seriously considered before (Figure 1). Therefore, it is highly demanded to develop new methods that allow us to understand and control the new states of electrons in terms of both experimental and theoretical solid state physics. Historically, the development of π-electron-based material has started from establishing the concept of 'organic semiconductors' by Prof. Inokuchi and it was followed by syntheses of many organic materials that exhibit metallic and even superconducting phases. After this first phase of material development, the second phase of π-electron material development has been led by physicists and physical chemists who have discussed band structures with coherent electrons, which had been hardly believed to exist in organics before those studies. In this context, we are now at the starting point of the third phase of π-electron-based solid state science. This new era requires researchers to develop new methods in all aspects of material development, observation/analytical method, and theoretical understanding. At the same time, it is necessary to facilitate interdisciplinary interaction among physicists, chemists, and device technologists to tackle this problem. This project aims at promoting such interdisciplinary discussions by holding a workshop with wide range of participants who share the common issues from different points of view.

During the workshop, it was recognized that the competition among energies with similar strengths can result in a situation of high complexity, yet such a complexity can generate unprecedented and interesting phenomena. In molecular materials, the energies of electron's motion, lattice, spin, and Coulomb interaction are at similar extent, and therefore mix together to form inhomogeneous but hierarchical structures in space and time domains. Theories now available seem to fail to help researchers understand and control such entangled situations. The participants agreed on the importance of developing new theories based on non-periodic structures, although complete removal of the periodicity is hard to be considered. The participants also agreed to continue this type of discussion and to propose a new research field that might be able to be called 'quantum π-ology'. Such a new science should result in understanding and control of strong correlation, glassy state, non-equibillium state, frustrated state, and ultra-fast transitions of π-electron systems in future. This project has succeeded to launch such a new research community that will pave the way to the third phase of π-electron science.

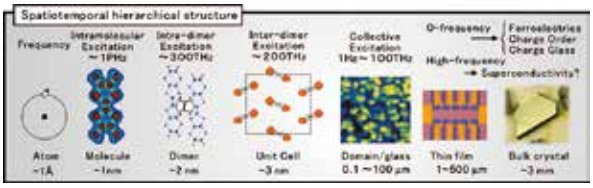

Figure 1. Spatiotemporal hierarchical structure of electrons and lattices in π-electron systems.

B. Catalysis Based on the Elemental Strategy

UOZUMI, Yasuhiro (*IMS*)
NAKAMURA, Masaharu (*Kyoto Univ.*)
KAKIUCHI, Fumitoshi (*Keio Univ.*)

Adhoc members
MURAI, Shinji (*Nara Inst. Sci. Tech.*)
TAMAO, Kohei (*RIKEN*)
MOMIYAMA, Norie (*IMS*)
OSAKO, Takao (*IMS*)
HAMASAKA, Go (*IMS*)

Rare resources, represented by rare earth and other rare metal elements which are being utilized for the advanced industries are facing their price increase and tight supply due to rapid increase of their consumptions and producing countries' resource management policies accompanying with the global economic growth and advanced industries' expansion.

In the past several decades, transition metal catalyses have been playing key role in the chemical industries to realize efficient organic molecular transformations, and rare and

noble transition metals (*e.g.* Pd, Pt, Rh, *etc*.) are often utilized as the central elements of the catalysts. Taking into accounts the above mentioned situations of elemental strategies, development of novel catalytic processes without rare and noble metals have been rapidly becoming an eagerly awaited research subjects.

This special project entitled "Catalysis Based on the Elemental Strategy" started in 2015 (one-year project) as a feasibility study to launch national-size research project of catalysis based on the elemental strategy. The three main proposers organized a study group by which the feasibility study meetings were held 3 times in 2015 (9^{th}–10^{th} of January (at Atami), 19^{th}–20^{th} of July (at Toyama), and 10^{th} October (at Okazaki)), and once in 2016 (23^{rd}–24^{th} January (at Yamaguchi)). Among them, the meetings at Atami, Toyama, and Yamaguchi were held with some adhok members, as a concomitant meeting of JST-CREST meeting on Elemantal Strategy (a representative: Prof. Kohei Tamao).

Through the thorough discussion on the feasibility, this study group decides to promote to make proposals of a couple of research projects related to this special project to MEXT and/or JSPS. Thus, a research project on developing an analytical system for elucidating the catalytic reactions utilizing synchrotron light sources *etc*. and that on developing novel catalytic systems, which would realize elemental-replacement, elemental-circulation, as well as elemental-reduction, will be proposed in due course.

(2) Research Symposia

(From Oct. 2015 to Sep. 2016)

Dates	Theme	Chair
Oct. 22, 2015	Workshop of Theoretical and Computational Molecular Science: Development of Computation Methods and Simulations	**YANAI, Takeshi**
Nov. 27, 2015	Emergence of Interaction and Hierarchy Hidden in Data	**HIRA, Ri-ichiro** **SHIKANO, Yutaka**
Feb. 11–12, 2016	Current and Future Status of Bright and Intense Infrared Light Source	**ZEN, Heishun** **KATOH, Masahiro**
Feb. 15–17, 2016	Japan-Korea Seminars on Biomolecular Science: Experiments and Simulation	**AONO, Shigetoshi**
Feb. 23–26, 2016	Japan-China Joint Symposium on Functional Supramolecular Architectures	**MAEDA, Hiromitsu** **JIANG, Donglin**
Mar. 5– 6, 2016	Materials Engineering Science with Asymmetric Coordination Sphere Design and Anisotropic Integration of Metal Complex	**SHIONOYA, Mitsuhiko** **MASAOKA, Shigeyuki**
Mar. 9–10, 2016	Molecular Catalysis Science: Interplay between Theory and Experiment	**HASEGAWA, Jun-ya** **EHARA, Masahiro**
Jun. 27–28, 2016	Engineering Super-Functional Molecules: Strategy for Design and Development of Socially Implementable Molecules Achieved by Cooperation among Synthesis, Measurement and Mathematical Analysis	**UENO, Takafumi** **IINO, Ryota**
Sep. 2– 3, 2016	Major Trends in Organometallic Chemistry	**HIRATA, Shuichi** **UOZUMI, Yasuhiro**
Sep. 29– 30, 2016	Japan-Korea-Taiwan Joint Symposium on Bioinorganic Chemistry	**AONO, Shigetoshi**
Jun. 26, 2016	Meeting for Lectures at 56^{th} Summer School on Molecular Science for Young Scientists	**MIZUNO, Yuta** **FURUTANI, Yuji**
Jan. 11–14, 2016	Tensor Network States: Algorithms and Applications 2016	**SHIKANO, Yutaka**

(3) Numbers of Joint Studies Programs

Categories		Oct. 2015–Mar. 2016		Apr. 2016–Sep. 2016		Total		
		Regular	NanoPlat	Regular	NanoPlat	Regular	NanoPlat	Sum
Special Projects		0		2		2		2
Research Symposia		7		4		11		11
Research Symposia for Young Researchers		0		1		1		1
Cooperative Research		30	33	37	36	67	69	136
Use of Facility	Instrument Center	7	70		74	7	144	151
	Equipment Development Center	2	7	1	5	3	12	15
Use of UVSOR Facility		61	20	65	21	126	41	167
Use of Facility Program of the Computer Center						217*		217*

* from April 2015 to March 2016