OKAZAKI CONFERENCES

The Sixty-Second Okazaki Conference

Structural Hierarchy in Molecular Science: From Nano and Meso Structures to Micro Structures (January 10–13, 1999)

Organizers: **AIDA, Takuzo** *(Univ. Tokyo)*
FUJITA, Makoto *(IMS)*

The precise construction of large structures in the range of 1–1000 nm is of great importance in modern science. For constructing these structures, we need to consider "structural hierarchy" in a molecular world. At the first step, we prepare molecules by conventional syntheses. Then the molecular building blocks are linked together into larger structures by covalent or noncovalent approaches. The covalent approach may involve the use of large molecular units (*e.g.*, porphyrin, C60, carborane etc.) or branched polymerization (dendorimer synthesis), whereas noncovalent synthesis requires templating and self-assembly exploiting weak bonds (*e.g.*, donor-acceptor interaction, hydrogen bond, coordination bond). To build up the next structural hierarchy (nano to meso structures), there seem to be little efficient methods. Thus we need to discuss and develop new concepts and methodologies (which could be chemical, physical, or biological). Finally, we also consider micro structures built up from molecules. Crystal engineering is a rapidly developed field which provides a powerful method for obtaining precise micro structures from molecules. However, completely different approaches to micro structures are still awaited. Such view points prompted us to organize a meeting which would bring together scientists active in a variety of fields: organic chemistry, inorganic chemistry, coordination chemistry, polymer science, material science, biochemistry, theoretical chemistry, *etc*. (that is to say, all fields in chemistry!) The following sessions were run in the conference with fruitful discussions.

- Molecular recognition - the first event for molecule-by-molecule syntheses
- Self-assembled nano structures
- Covalent approaches to nano structures: New class of polymers and dendrimers
- Function of nano structures
- Toward meso structures
- Precise control of micro structures: Crystal engineering
- Bio-related nano structures
- Perspective

The Sixty-Third Okazaki Conference

Laser Spectroscopy of Molecular Clusters — Structure and dynamics— (March 23–25, 1999)

Organizer: **EBATA, Takayuki** *(Tohoku Univ.)*
FUJII, Masaaki *(IMS)*

Invited Overseas Speakers:
LEUTWYLER, S. *(Univ. Bern)*
NEUSSER, H. J. *(Tech. Univ. München)*
ALBRECHT, A. C. *(Cornell Univ.)*
TOPP, M. *(Univ. Pennsilvania)*
XANTHEAS, S. S. *(Pacific Northwest Lab.)*
KLEINERMANNS, K. *(Univ. Düsseldorf)*
LAENEN, R. *(Tech. Univ. München)*
WEINKAUF, R. *(Tech. Univ. München)*
DEDONDER-LARDEUX, C. *(Univ. Paris-sud Orsay)*
PARMENTER, C. *(Indiana Univ.)*

Molecular clusters in which molecules are bound by a weak inter-molecular force such as hydrogen bond or van der Waals force have been extensively studied since they provide us a detailed information of the inter-molecular potential. The information is quite useful to the investigation of the local structure and the vibrational relaxation in condensed phase. Furthermore, it may be possible to find new chemical reactions and them by use of the molecular clusters. However, it is quite recent that the cluster structures are accurately determined experimentally and theoretically. The purpose of the 63rd Okazaki conference was to present recent progress of laser spectroscopy and theory to reveal the structures and the dynamics of not only neutral but also ionic clusters.

We focused our attention on three subjects in this conference. First is that to what extent the recent laser spectroscopic methods become powerful to determine the structure of the clusters. Second is the recognition how the recent theory, especially ab initio molecular orbital calculation, plays an important role for the determination or the prediction of the cluster structures. Third is that how our knowledge of molecular clusters can be applied to the problem of the condensed phase.

In the conference, 10 invited foreign speakers and 14 Japanese speakers gave excellent talks and 28 posters are presented. In spite of tight schedule, we had stimulated discussions. Many laser spectroscopic methods, that is mass-selected REMPI, MATI, ZEKE, photoelectron, population labeling, and double resonant vibrational spectroscopies were introduced. We saw how the electronic and vibrational spectra of an isolated molecule change upon the cluster formation and discussed how the spectra are compared with the structures predicted by ab initio calculations. The experimental studies on the dynamics of electronically and vibrationally excited clusters were presented. We also understood that in condensed phase the redistribution of the energy to the first shell molecules is the first step of the vibrational relaxation. In that sense, we again realized the importance of the communication between the scientists studied on clusters and on condensed phase.

Okazaki COE Conference

High Resolution Spectroscopy of Molecules and Atoms: Present Status and Future Trends
(March 17–19, 1999)

Organizing Committee:
SAITO Shuji; MORITA Norio; KATO Tatsuhisa
(Department of Molecular Structure)

The Institute for Molecular Science (IMS) has been recognized as a Center of Excellence (COE) officially by the Ministry of Education, Science, Culture, and Sports of Japan. By the financial support from the Ministry we have an opportunity to organize an international symposium within this Japanese fiscal year.

Considering the recent remarkable experimental progress in the highly resolved spectroscopy of molecules and atoms not only in gass phase but also in condensed phase, we have determined the title of the symposium as "High Resolution Spectroscopy of Molecules and Atoms: Present Status and Future Trends." The symposium was held from March 17 (Wed) through 19 (Fri) in 1999 at the Okazaki Conference Center.

Recent experimental progress in the related various field of the highly resolved spectroscopy is remarkable, and we think that it is really timely and valuable to organize such a symposium to stimulate interdisciplinary information exchange and discussions and to promote further developments. We covered the following subjects: (1) Microwave spectroscopy of transient molecules, (2) Laser spectroscopy of molecules and atoms, (3) high resolution spectroscopy in solid.

Twenty five invited talks and twenty eight posters were presented, and about 100 people attended the conference. Very fruitful discussions were made among the different fields of the spectroscopy. The conference was very successful. The interdisciplinary discussions were stimulated and the further developments would be promoted.