AWARDS

Professor Kaya's Scientific Achievements

Professor Koji Kaya, Director General of Institute for Molecular Science, received the Chemical Society of Japan Award in 2000 for his contribution to "Creation and Development of Cluster Chemistry—Composite Effects in Binary Components." Clusters, intermediate states of matter between the bulk and gas phases, have gained much attention recently as one of the key materials in nano-science. Professor Kaya has opened up new research field of cluster chemistry by focusing his attention on the composite effects observed in binary clusters. His scientific achievements relevant to the award are summarized as follows.

1) Investigation of electronic and geometrical structures of clusters of metal and semiconductor. He has developed a new diagnostics for the structures of the clusters based on extremely sensitive photoelectron spectroscopy and chemical doping method. One of the most important findings is that origin of photoluminescence from the semiconductor clusters is not due to the quantum size effects but to the surface oxide layers.
2) Production of novel organometallic clusters. Numbers of inorganic/organic hybrid clusters, having "sandwich" structures, have been prepared by laser vaporization of bulk metal in the presence of organic molecule. He has also developed a new method to deposit these novel clusters onto substrate without dissociation (soft landing method), which will be a powerful and promising technique to produce variety of cluster–assembled materials.

Professor Fumio Hirata

Professor Fumio Hirata of Department of Theoretical Studies won the Scientific Award of the Chemical Society of Japan in 2000 for his contributions to "Development of New Molecular Liquid Theory in Chemistry and Its Application." Professor Hirata's scientific achievements relevant to the award are summarized as follows:

1. Development of extended RISM theory.
   Although the original version of the reference interaction site model (RISM) theory enabled one to incorporate the effects of molecular geometry into the liquid theory, it was incomplete in the sense that it cannot deal with the electrostatic interactions. Professor Hirata extended the theory so that these interactions can be included. This is important because electrostatic interactions are essential in describing chemistry occuring in solution. His theory enabled researchers for the first time to study organic solvent, alcohol, and water in a quantitative manner.
2. Development of RISM-SCF theory.
   In quantum chemistry field the effects of solvent were usually included by continuum dielectric models. Professor Hirata developed the so-called RISM-SCF theory in which the effects of solvent on the electronic structure are incorporated by the RISM theory. The theory determines the electronic structures of solute and microscopic structures of solvent in a self-consistent manner.
3. Study of microscopic structures of liquid and its dynamics.
   Dynamics of liquid had been studied traditionally by spherical molecular models or those with embedded multipoles. Professor Hirata introduced the interaction-site description to liquid dynamics, which enables one to study dynamics of much more realistic system of chemical interests such as water and alcohol.
4. Study of electrode surface-solvent interactions and statistical mechanics of electrode reactions.
   Modern experimental techniques including STM, AFM, and SEIRAS have been revealing the electrode-solution interface in atomic detail, so that the current theories of electrode represented by the Gouy-Chapman double-layer theory is becoming senseless. By combining extended RISM, polymer RISM, and the density functional theory, Professor Hirata has been constructing a theory which is capable of exploring the electrode-solution interface in the same resolution as in the experimental methods. The theory allowed him to successfully study water structures near the electrode surfaces, electronic structures, and nonlinearity of charge transfer reactions.
5. Study of stability of biopolymers in solution and protein folding problem.
   Effects of solvent play an essential role in the stability of biopolymers in solution. Professor Hirata has been studying the elements of the stability from the physical-chemical viewpoint. In particular, he proposed to combine molecular simulations with extended RISM theory of solvation and also with extended scaled particle theory of solvation. He has given quantitative accounts of solvation effects on the stability of biomolecules as functions of tempearture, pressure, and ion concentration, etc. These studies give much information in the protein folding problem.

Professor Akasaka's Scientific Achievements

Professor Takeshi Akasaka, Department of Molecular Structure, received the Scientific Award of the Chemical Society of Japan in 2000 for his contribution to "Organic Chemistry of Fullerenes," and the Award of the Niigata Nippou in 2000 for his contribution to "Exohedral and Endohedral Chemistry of Fullerenes." Since the success of laboratory synthesis of C_{60} and other fullerenes, their chemical derivatives have been reported within a decade. Especially metallofullerenes (fullerenes with metal(s) inside the hollow spherical carbon cage) have interested people because of their possibilities of the free tune of "outside chemistry," and have been prepared and characterized. The electronic structure might reflect the chemical reactivity of metallofullerenes. Professor Akasaka has found a new photochemical exohedral derivatization of typical empty fullerenes such as C_{60} and C_{70} with disilirane. Moreover, he has found the chemical derivatization of endohedral metallofullerenes, La@C_{82} and Gd@C_{82} with disilirane. Recently he found that the anion of La@C_{82} had a unique stability toward air and water, and determined the molecular structure of the La@C_{82} anion by means of ^{13}C-NMR spectroscopy.

Professor Aida's Scientific Achievements

Professor Takuzo Aida (Department of Chemistry and Biotechnology, Graduate School of Engineering, The University of Tokyo), a visiting professor of Coordination Chemistry Laboratories (1999–2000), received "Nagoya Medal Seminar: Silver Medal Award 2000" and "Tokyo Techno Forum: Gold Medal Award 2001," for his outstanding contribution to "Design and Functions of Macromolecular and Supramolecular Materials." His scientific achievements relevant to these awards are summarized as follows.

1. Development of light-harvesting dendritic macromolecules and their nanoscopic photochemical and physical properties.
2. Development of a novel bioinspired fabrication of advanced polymeric materials by using mesoporous silicate materials.
3. Development of chirality-memory supramolecular systems for sensing asymmetric molecules.

Associate Professor Takasu's Scientific Achievements

Associate Professor Masako Takasu of Department of Applied Molecular Science received Molecular Simulation Award from the Molecular Simulation Society of Japan for her contribution to "Simulation of Quantum Systems in Random Media."

Her scientific achievements relevant to the award are summarized as follows.

1. Quantum calculations of electron in random media.
2. Simulation of superfluid transition of helium in random media.

This award is given annually to prospective scientists under 41 years old who made outstanding contribution in the area of molecular simulation.

Associate Professor Tahara's Scientific Achievements

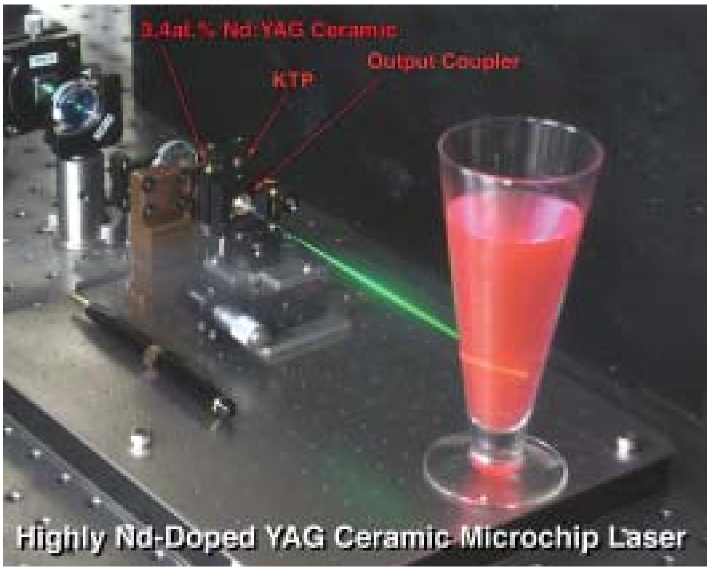
Associate professor Tahei Tahara of Department of Vacuum UV Photoscience received the TRVS Outstanding Young Researcher Award (2001) for his contributions to "A new observation and a new method in time-resolved Raman spectroscopy." This award was given to the outstanding researchers who presented excellent scientific results in the 10th TRVS (Time-Resolved Vibrational Spectroscopy) international conference held at IMS in May, 21–25, 2001. In his invited talk, professor Tahara presented two new achievements in time-resolved Raman spectroscopy. First, he reported a picosecond Raman study of the local solvating structure around an electron injected in water (solvated electron). The solvated electron is the most fundamental ionic species in solution, and hence, the ultrafast dynamics has been extensively studied so far through time-resolved measurements of its electronic $p \leftarrow s$ transition appearing in the near-infrared region. However, the local solvating structure cannot be unveiled by such an electronic spectroscopy. It is highly desirable to directly observe vibrational spectra of the water molecules that solvates the electron. He found that a transient Raman band appears in the OH bending region, when Raman spectra of water were measured under a probing condition resonant with the $p \leftarrow s$ transition of the solvated electron. He successfully attributed the observed Raman signal to the solvating water molecules that strongly interact with the electron, and clarified the local structure of the water molecules in the solvation shell. The second topic was about the development of a new spectroscopic method for the study of low-frequency vibrations. In time-resolved Raman measurements using multichannel detectors, it is practically quite difficult to measure spectra in the low frequency region because of the disturbance of a strong Rayleigh scattering. In his efforts to overcome this difficulty, he has developed a novel method to study the low-frequency vibrations of short-lived transient species by utilizing a time-domain Raman spectroscopy (impulsive stimulated Raman scattering, ISRS) as the probe process in time-resolved Raman measurements. Making the most use of this method, he recently succeeded in measuring ISRS signals of an excited-state polyatomic molecule in solution.

Associate Professor Mitsuke's Scientific Achievements

Associate professor Koichiro Mitsuke of Department of Vacuum UV Photoscience received the BCSJ Award of the Chemical Society of Japan in 2001 for his contribution entitled "UV and visible emission spectra from photodissociation of OCS using synchrotron radiation at 15–30 eV" published in the Bulletin of the Chemical Society of Japan. This work was fully accomplished at the UVSOR facility of IMS.

Professor Mitsuke has developed a new method of fluorescence spectroscopy by combining monochromatized undulator radiation with high sensitive imaging spectrograph. This method allows one to investigate various decay dynamics of transient superexcited states embedded in multiple dissociation continua. Professor Mitsuke has newly identified many electronic transitions and emission band systems arising from photodissociation of OCS. He has succeeded in presenting two powerful and complementary methods for gas-phase photoionization and photodissociation studies in the extreme UV region, *i.e.* two-dimensional photoelectron and fluorescence spectroscopies, both of which have been developed in the UVSOR facility.

Associate Professor Taira's Achievements



Associate professor Takunori Taira of Laser Research Center for Molecular Science received the promotion award of metal-structure photographs from the Japan Institute of Metal in 2001. This award was give to photographs of academic and technological excellence and the title of his award is "YAG ceramics for high-power laser oscillation." The award is shared with his collaborator, Dr. Ikesue of Japan Fine Ceramics Center, and their several-years achievements are widely accepted.

A cost effective and moldable ceramic material is inspiring into solid-state lasers emitting 1 μm wavelength although single crystal Nd:YAG is conventionally utilized in laser systems. Nd:YAG crystal is usually grown from liquid phase by the Cz method and growth speed is limited up to several mm/h to maintain crystal quality, which is an obstacle to low-cost and large-scale growth. It is difficult to increase concentration of active Nd ions more than 1.4 at.% in the method because the crystal passes the liquid phase during growth. Low concentration is a drawback of single crystal Nd:YAG for achieving a microchip laser due to insufficient pump absorption. This is a main reason to use Nd:YVO_4 with high absorption coefficient in microchip lasers although it has low thermal conductivity.

Professor Taira and Dr. Ikesue have been pursuing a growth technique of Nd:YAG and discovered a sintering method for obtaining transparent ceramics with high Nd density, which lead to the first ceramic-based microchip laser. The figure shows a highly Nd-doped YAG ceramic microchip laser emitting 532 nm green light through wavelength conversion. This is a clear evidence of low scattering loss in laser materials allowing wavelength conversion even in a cavity. The ceramic technique will open the way to selective doping of active and saturable ions for integration of multifunctions.

Associate Professor Iwata's Scientific Achievements

Associate professor Koichi Iwata, Department of Applied Molecular Science, received the Morino Science Award in 2000 for his contributions to "Development of time-resolved infrared and Raman spectroscopic methods and modeling of ultrafast reaction dynamics in solution." Time-resolved vibrational spectroscopy is very crucial for the study of the structure and dynamics of short-lived transient species. Professor Iwata has been making pioneering contributions to the development of time-resolved vibrational spectrometers, such as a microsecond infrared spectrometer using a dispersive monochromator as well as a picosecond Raman spectrometer combined with a high-repetition-rate laser system. These spectrometers have enabled us to sensitively detect vibrational bands of the transient species, which is essential for the full elucidation of the chemical reaction dynamics. It can be said that these methods are now the most standard and popular system for the physicochemical study of the dynamical properties of molecules. Professor Iwata's achievements that have been made using these spectrometers are summarized as follows. (1) microsecond infrared study of the generation and annihilation dynamics of charged solitons in polyacetylene films, (2) picosecond Raman study of the vibrational cooling dynamics of S_1 *trans*-stilbene, which was then extended to (3) the elucidation of the solute-solvent energy transfer dynamics, (4) characterization of bimolecular reactions between aromatic compounds and solvent carbon tetrachloride by time-resolved infrared and visible absorption studies, and (5) modeling of the translational motion of solution-phase molecules in terms of the statistical diffusion in the picosecond time region.

Research Associate Mizutani's Scientific Achievement

Dr. Yasuhisa Mizutani, a research associate in Laboratory for Molecular Dynamics, Department of Molecular Structure, received the 17th Morino Science Award for his contribution to "Time-resolved Resonance Raman Studies of Photochemical Reactions in Solutions and Vibrational Energy Relaxation." Throughout his career he has been interested in structure and dynamics of complex systems such as liquids and proteins. When he joined IMS as a research associate, he decided to do some new experiments to answer a question, 'How do surrounding solvent molecules respond to a step-function like structural change of a solute molecule?' Practically, he planned to investigate the energy and structure relaxation of solute molecules using time-resolved vibrational spectroscopy, and started from the construction of a light source for measuring picosecond pump/probe time-resolved resonance Raman spectra with kiloheltz repetition in which the pump and probe wavelengths could be tuned independently. After a few years he succeeded in observing anti-Stokes time-resolved resonance Raman spectra of photodissociated carbonmonoxy myoglobin and unraveled the cooling dynamics of heme heated by photodissociation. The results were published in Science. Furthermore, he demonstrated that the expansion of porphyrin due to the low- to high-spin transition of iron occurs within 1 ps, but its out-of-plane movement and subsequent change of protein structures take place around ~10 ps and ~100 ps, respectively. On the other hand, he also investigated vibrational energy relaxation of metalloporphyrins in solutions and observed the vibrational energy redistribution process in a picosecond time regime. He pointed out the mode dependence of the vibrational relaxation for metalloporphyrins and heme proteins. Thus, he opened a new route to study molecular dynamics in solutions.

Dr. Hiroshi Noguchi's Scientific Achievements

Dr. Hiroshi Noguchi, a JSPS postdoctoral fellow in Takasu Group at the Department of Applied Molecular Science, received the Award for Encouragement of Research in Material Science in December 2000 for his contribution on "Electophoretic Behavior of Polyelectrolytes in Gel and Polymer Solutions."

This award is given to young scientists (under 36 years old) who made contribution in the area of material sciences and gave excellent presentation at the Annual Symposium of MRS-Japan.