AWARDS

Professor Emeritus Kaya's Scientific Achievements

Professor Emeritus Koji Kaya, the former Director General of IMS, was selected as "the Person of Cultural Merit in 2005" for his outstanding contributions to "nano-materials science."

Professor Kaya started his scientific carrier with an aim to understand the details of interaction between atoms and molecules. He has determined the structures of van der Waals complexes precisely by high-resolution laser spectroscopy. On the basis of the fundamental knowledge of intermolecular interaction, he has devoted himself to the research of clusters, aggregates of atoms and molecules. Various types of molecular assemblies with novel structures and properties have been produced size selectively by using laser vaporization and molecular beam techniques. One of the representative systems is a one-dimensional organo-metallic cluster, in which metal atoms and organic molecules are stacked alternately. Unique behavior of the electrons within these "sandwich clusters" has gained wide interests from both experimental and theoretical viewpoints. These clusters are potential candidates of building blocks of functional nano-materials. He has developed a method, referred to as a soft-landing method, to assemble these unique clusters onto a surface, which will open the door to a new research field of nano-materials science.

As described above, Professor Kaya has played a significant role as a forerunner in establishing a new research field of nano-materials science.

Professor Emeritus Tanaka's Scientific Achievements

Dr. Ikuzo Tanaka, former president and professor emeritus of Tokyo Institute of Technology, received the Person of Cultural Merit for 2005 in recognition of his contributions to both research and education in the field of physical chemistry, in particular photochemistry. He made outstanding research achievements and fostered many excellent scientists. He also contributed greatly to enhancement of higher education serving as the president of academic organizations including Tokyo Institute of Technology and the National Institution of Academic Degrees.

Having started the photochemistry research in 1950's, Dr. Tanaka was one of the pioneers in the field. He initiated development of photoionization mass spectrometry by utilizing the vacuum ultraviolet light irradiation in stead of conventional electron impact. This original work was highly evaluated in the international scientific community. He also introduced using lasers in the chemical research. The laser-driven pump and probe method resulted in improvement of energy and time resolution for the studies of excited state creation and chemical reactions.

Dr. Tanaka devoted himself to the advancement of the study. He took leadership in founding a new academic society on photochemistry: the Japanese Photochemistry Association, and was selected as the first president. His presidency in other academic societies includes the Chemical Society of Japan and the Japan Society of Energy and Resources. In addition, he chaired many domestic and international scientific committees.

Japan is one of the world-leading states in photochemistry with the highest standards of research in both basic and applied fields such as functional materials, environment, energy, and information and communication technology. Dr. Tanaka, as a pioneer and front-runner of the research, played an important role in promotion of science and human development.

Dr. Tanaka received Order of the Rising Sun with Gold and Silver Star in 2001, Medal with Purple Ribbon in 1989, Toray Science and Technology Prize in 1985, The Chemical Society of Japan Award in 1977, The Matsunaga Prize in 1970, and The Chemical Society of Japan Award for Young Chemist in 1959.

Professor Kobayashi's Scientific Achievements

Prof. Hayao Kobayashi of the Department of Molecular Assemblies received a Chemical Society of Japan Award in 2006 for his contributions to "Studies on Magnetic Organic Superconductors and Single-component Molecular Metals." By highly sophisticated physical measurements, Prof. Kobayashi have developed various new functional molecular materials such as magnetic organic superconductors and single-component molecular conductors. The followings are the summary of his scientific achievements related to the award.

1) Magnetic Organic Superconductors

Itinerant and localized hybrid spin systems are candidates for possible new cooperative phenomena. However, most of the researches could not obtained functions beyond those of individual spin species. Prof. Kobayashi focused on BETS, bis(ethylendithiolo)tetraselenafulvalene, molecules, and discovered field induced organic superconductors in λ-$(BETS)_2FeCl_4$, λ-$(BETS)_2Fe_xGa_{1-x}Cl_4$, κ-$(BETS)_2FeBr_4$. This observation is beyond our expectation since

superconducting phases are not stable under magnetic filed. By a series of researches following this, he discovered new phenomena such as colossal magneto-resistance effects and noble metal-superconductivity-insulator transition. They are cooperative phenomena which cannot be realized by the individual conduction electron and magnetic ion. He established the new field "magnetic organic conductors."

2) Single-component Molecular Metals

Conventional organic conductors are composed of two components to create conduction electrons. So single-component molecular metals like copper or gold has been one of the chemist's dreams. Prof. Kobayashi and co-worker focused on the system which possesses significant three-dimensional inter-molecular interactions and a small HOMO-LUMO gap, and developed a series of the π extended transition metal complexes. Prof. Kobayashi developed the first single-component molecular metals based on the transition metal with extended-TTF ligands, $Ni(tmdt)_2$ and $Au(tmdt)_2$. After this discovery, extensive investigations for single-component molecular metals are performed. The very precision magnetization measurement under a strong magnetic field revealed the existence of the Fermi surface, which is a clear evidence of metal. The evaluated cross-section of the Fermi surfaces are coincided with the first-principle calculation result. The metallic properties of these single-component molecular metals are considered to be realized as compensated-metals such as Mg or Al. This discovery just realizes the dream which chemists are giving up, has big and international influence also on a lot of researchers.

These achievement mentioned here captured the high spotlight internationally from a viewpoint of new functionality molecular materials.

Professor Matsumoto's Scientific Achievements

Professor Yoshiyasu Matsumoto received "The CSJ Award for Creative Work" in the spring of 2006 from Chemical Society of Japan for his achievements on "Ultrafast dynamics in surface photochemistry."

Photocemistry at well-defined surface is an important subject from the viewpoint of application such as photocatalysts as well as fundamental science. Professor Matsumoto has investigated dynamics of photochemical processes by employing time-resolved non-linear spectroscopy. The major achievements are (1) elucidation of the excitation mechanism in photochemistry of adsorbates on surfaces, (2) real-time probing of dynamics of electron transfer and (3) photo-induced nuclear dynamics at surfaces. These achievements have contributed to the development of new areas in surface science and related research fields such as nanoscience and photoscience.

Dr. Tahara's Scientific Achievements

Dr. Tahei Tahara, Chief Scientist of Molecular Spectroscopy Laboratory, RIKEN (Institute for Chemical Research), a former associate professor (1995–2001) of Department of Vacuum UV Photoscience, IMS, has been awarded the Japan Society for the Promotion of Science Prize in 2005 for his contribution, "Studies of Molecular Dynamics in the Condensed Phase by Ultrafast Time-Resolved Spectroscopy." Dr. Tahara has performed systematic studies on the real-time observation on the intramolecular nuclear dynamics in ultrafast photoreaction, such as unimolecular dissociation, proton transfer, isomerization, by developing novel techniques/instruments. All his recent scientific accomplishments have made a large contribution to the deep understanding of elementary processes in photochemical reactions in condensed phase.

Associate Professor Donglin Jiang's Scientific Achievement

Professor Donglin Jiang of Department of Applied Molecular Science received two awards. One is the *Young Scientist Award* from the Minister of Ministry of Education, Culture, Sports, Science and Technology of Japan (MEXT). The award title is "Study of functional nano-materials in polymer science." Another one is the *Wiley Award* from the Society of Polymer Science, Japan. The award title is "Synthesis and functions of polymers with tree-like morphology." Both awards are given for the original synthetic work on dendrimer. Dr. Jiang synthesized various kinds of highly functional materials employing nano-scale molecule called a dendrimer, which consists of core and dendron. First, he synthesized a heme-dendrimer with iron porphyrin as the core, and demonstrated that this molecule reversibly absorbs and desorbs oxygen molecules. Second, he synthesized a spherical dendrimer that works as a light-harvesting antenna. This finding has drawn much attention of all material scientists around the world. Third, he synthesized a columnar dendrimer that acts as a highly efficient catalyst for the generation of hydrogen molecules through the photo-reduction of water molecule. Fourth, he synthesized an amphiphilic dendron with photo-functional groups, and found that the dendrons are self-assembled to form a nano-scale organic tube with a narrow size distribution. Since the tube consists of a donor and acceptor layers, a highly efficient photoconduction is

expected. Fifth, he synthesized a polymer iron complex with dendron-type ligands. This complex changes the spin state of the iron ion depending upon the temperature. As described above, the work of Dr. Jiang has given a strong impact to the field of material science.

Associate Professor Morita's Scientific Achievement

Prof. Akihiro Morita, Department of Computational Molecular Science, received the Morino Science Award in 2006 for his contributions to "Theoretical study on structure and dynamics of solutions and solution interfaces." He has made pioneering contributions to solution chemistry and heterogeneous chemistry associated to liquid interfaces and atmospheric aerosols, using ab initio electronic structure theory and molecular dynamics simulation.

He has developed an ab initio theory of electronic polarization, called the charge response kernel, and thereby elucidated several mechanisms of experimental novel phenomena, including diffusion of radical species and vibrational relaxation of azide ions, where the electronic polarization turned out to play crucial roles. In the field of heterogeneous chemistry, one of the most noticeable achievements is the development of theory and first-principle computational methods of vibrational sum frequency generation (SFG) spectroscopy. This work opened a new avenue of detailed and unambiguous analysis of SFG spectra with the help of molecular simulation.

Associate Professor Tsukuda's Scientific Achievement

Associate Professor Tatsuya Tsukuda of Research Center for Molecular-Scale Nanoscience was awarded for best oral presentation at the GOLD2006 conference (September, 2006). The title of his paper was "Polymer-stabilized gold clusters as quasi-homogeneous catalysts for aerobic oxidation in water." He demonstrated that the gold clusters stabilized by polymer act as efficient catalysts for aerobic oxidation of alcohols in water and that the activity is increased with decrease in size. The size-dependent activity was explained in terms of quasi-molecular electronic structures of the small clusters.

Research Associate Dr. Hatsui's Scientific Achievement

Research Associate Dr. Takaki Hatsui of Department of Vacuum UV Photoscience has received the Japanese Society for Synchrotron Radiation Research (JSSRR) Award 2006 for his contribution to the promotion of synchrotron radiation research in January 2006. The title of his work is "Development of a Novel High-Resolution Spectrometer for Soft X-ray Emission Studies." His design consists of a Wolter type I mirror, a free-standing transmission grating, and a back-illuminated CCD, and is completely different from conventional types of soft X-ray emission spectrometers. His spectrometer can achieve >5000 ($E/\Delta E$) energy resolution; on the other hand, a typical energy resolution of conventional ones is <2000. His spectrometer will be a most-promising one for the next-generation soft X-ray emission spectrometer using high brilliant synchrotron radiation.

Research Associate Dr. Higashibayashi's Scientific Achievement

Dr. Shuhei Higashibayashi, Research Associate of Research Center for Molecular-Scale Nanoscience, received the Young Scientist's Research Award in Natural Product Chemistry in the 40th Young Scientist Meeting on Natural Product Chemistry (2005) for his contribution to "Creation of Universal NMR Database for the Stereochemical Assignment of Acyclic Natural Products." This award is given to a young scientist (younger than 34 years of age) who has made notable contributions to the field of natural product chemistry or bioorganic chemistry. Dr. Higashibayashi developed Universal NMR Database approach to determine the stereochemical configurations of acyclic organic molecules. This methodology realized direct determination of the stereochemical configurations of acyclic organic molecules with the ^{1}H and ^{13}C chemical shifts and the vicinal $^{1}H/^{1}H$ spin-coupling constant of NMR spectra without chemical degradation or derivatization. Universal NMR Database can be applied to any acyclic organic molecules and determine the stereochemical configurations of the corresponding common structural units in the molecules at once. Universal NMR Database approach has been already utilized for the stereochemical assignment of many natural products.

Research Associate Dr. Negishi's Scientific Achievement

Dr. Negishi, a research associate of Research Center for Molecular-Scale Nanoscience, received the Best Young Presenter Award for the presentation of an Excellent paper in the 4th Annual Meeting of Society of Nano Science and Technology. The title of the paper was "$Au_{25}(SR)_{18}$: discovery and the origin of the stability." He established precise synthesis method of thiolated gold (Au:SR) clusters, based on polyacrylamide gel electrophoresis and electrospray ionization mass spectrometry. Among various Au:SR clusters thus synthesized, it was found that the $Au_{25}(SR)_{18}$ clusters exhibit extraordinarily high stability against size-reducing processes. He also developed a large-scale synthesis method for Au_{25} clusters utilizing the high stability against thiol-mediated etching.

Research Associate Tanaka's Scientific Achievement

Dr. Hirofumi Tanaka, Research Associate of Research Center for Molecular Scale Nanoscience, received the Best Young Presenter Award for the presentation titled "Porphyrin Molecules Working as Nanodevice on Single-walled Carbon Nanotube" in the 4th annual meeting of Society of Nano Science and Technology held in Kyoto University.

He succeeded to fabricate the arrangement of 2-3-nm-size porphyrin aggregations adsorbed on single-walled carbon nanotube (SWCNT) using self-assembly. He also succeeded the direct measurement for the electric property of each aggregation by newly developed method of Point-contact Current Imaging (PCI-) AFM. Results showed that *I-V* curves on the exposed SWCNT were symmetric with respect to the origin but that through the porphyrin aggregation was asymmetric. The results indicate that the porphyrin aggregation on SWCNT works as a nano-rectification device which is one of the smallest organic devices at the present time. These results will assist to develop the new field of molecular electronics and nanoelectronics.

Dr. Iwahashi's Scientific Achievement

Dr. Iwahashi received the poster prize of Annual Meeting of EMLG/JMLG 2005 held in Prague on September 4–8, 2005. The poster was entitled "Molecular dynamics study of extension of α-helical peptides."

Extension-force curves for polyalanine and polyglutamic acid in water have been calculated based upon molecular dynamics calculation combined with thermodynamic integration method. The calculation is of higher accuracy than that obtained by other conventional methods such as steered MD. Based upon this method, he successfully showed a molecular picture for the force which originates in conformational entropy of the peptide chain.

Dr. Tsunoyama's Scientific Achievement

Dr. Hironori Tsunoyama, an IMS fellow in Research Center for Molecular-Scale Nanoscience, received Best Young Presenter Award in the 4th Annual Meeting of Society of Nano Science and Technology (May, 2006). The title of his paper was "Isolation of Alkanethiolate-Protected Au_{55} Clusters by Recycling Gel Permeation Chromatography (GPC)." He succeeded in synthesis of alkanethiolate-protected Au_{55} clusters by size separation with recycling GPC out of the crude samples prepared by thiolation of polymer-stabilized Au clusters. The newly prepared Au_{55} provides a prototypical system for fundamental study of nano-scale material and application in nano-device.

Mr. M. Fuyuki's Scientific Achievement

Mr. Masanori Fuyuki, a graduate student of SOKENDAI, received the Student Award for the presentation of an excellent poster entitled "Excitation mechanism of coherent phonons on alkali-metal adsorbed metal surfaces" in the 46th IUVSTA Workshop & 5th International Symposium on Ultrafast Surface Dynamics, which was held at Abashiri in 21–25 May 2006. He performed observations of coherent phonons on alkali-metal on metal surfaces by femtosecond time-resolved second harmonic generation. He succeeded in measuring the action spectra of coherent amplitude as a function of photon energy of pump pulses in Na/Cu(111) and K/Pt(111) adsorption systems, which allowed him to pin down the excitation mechanism for the coherent phonons.

Graduate Student Shiratori's Scientific Achievement

Mr. Kazuya Shiratori, a graduate student of Department of Structural Molecular Science, School of Physical Sciences, The Graduate University for Advanced Studies, received the Young Scientist Award for the presentation of an excellent paper in the 22nd Symposium on Chemical Kinetics and Dynamics (June, 2006). The title of the paper was "Electronic structure calculations of adsorbate-surface systems based on finite-temperature density functional theory." He developed the method of quantum chemistry calculations based on finite temperature density functional theory to describe the electronic structures of (sulfur-gold) adsorbate-surface systems. He investigated the electronic structures depending on temperature and the size of the cluster model.

Graduate Student Yoshimura's Scientific Achievement

Mr. Hideaki Yoshimura, a graduate student of Department of Structural Molecular Science, School of Physical Sciences, the Graduate University for Advanced Studies received the Graduate Student Award for the Presentation of an Excellent Paper in the Annual Meeting of The Chemical Society of Japan held on March, 2006. The title of his paper was "Selective Oxygen Sensing Mechanism in the Oxygen Sensor Protein HemAT by means of hydrogen bonding network." 85 papers were selected for this award out of 290 of the applications.