# AWARDS

## Professor Nakamura

Professor Hiroki Nakamura of Department of Theoretical Studies won the “Chunichi Culture Prize” in 2000 for his establishment of the fundamental theory of nonadiabatic transition due to curve crossing. Nonadiabatic transitions are well known to play crucial roles in various fields of physics, chemistry, and biology as one of the most important mechanisms of state and/or phase changes. Since the pioneering works done by Landau, Zener, and Stueckelberg in 1932, many investigators challenged to complete the theory with no full success. Professor Nakamura has also been working on the subject over twenty years, and recently he finally succeeded in obtaining the complete solutions of the Landau-Zener-Stueckelberg curve crossing problems in collaboration with his graduate student, C. Zhu. This theory provides the accurate compact formula for nonadiabatic transition probability, which replaces the celebrated Landau-Zener formula completely. Besides, it furnishes a complete set of accurate compact expressions for probabilities and phases to treat not only the Landau-Zener type but also the nonadiabatic tunneling type curve crossing problems. His research is thus evaluated as creating the fundamentally important aspects of nonadiabatic transitions, and it is expected that the theory would open up useful applications to a wide range of physical and chemical problems.

## Professor Iwata’s Scientific Achievements

Professor Suehiro Iwata of Theoretical Division received the Chemical Society of Japan Award in 1999 for his contribution to “Developments of Molecular Orbital Theory and Applications to Molecular Science.” His scientific achievements relevant to the award are summarized as following.

1. Developments of effective Hamiltonian theory. He has developed new method of effective Hamiltonian in Fock-space representation, and proved that the semi-empirical formalism can be derived from his method.
2. Theoretical studies on electronic excited states and ionized states. He has developed “Valence vacant orbital method” to describe electronic excited states and ionized states. He applied his method to the assignments of photoelectron spectra and characterization of highly excited electronic states.
3. Theoretical contribution to Cluster Science. He has applied the Quantum Chemistry methods to the analysis of structure, reactivity and spectroscopy of molecular clusters, i.e., metal cluster, phenol-water system, and anionic states of water cluster. Especially, he has discovered that electronic structure of water cluster anion can be characterized as “electron-hydrogen bonding,” where a diffuse anionic orbital has new type of hydrogen bonding nature with surrounding H–O group.

## Professor Watanabe’s Scientific Achievements

Professor Yoshihito Watanabe, Department of Applied Molecular Science, received the Scientific Award of the Chemical Society of Japan in 1999 for his contribution to “Elucidation of Molecular Mechanism for the Formation of High Valent Oxidative Intermediates in Heme Enzymes.” Proteins containing the heme prosthetic group catalyze various kinds of oxidation and oxygenation reactions. Prof. Watanabe’s studies aim to elucidate structure-function relationship of the protein moiety in activation of the O–O bond of peroxides. He focused his attention on the formation and decay mechanism of so called compound I intermediate, which should have an oxidized heme including $O{=}Fe^{V}$ Por, $O{=}Fe^{IV}$ $Por^{+\bullet}$, $Fe^{III}Pro^{++}$, $O{=}Fe^{IV}$ Por + amino acid cation radical, $ROO{-}Fe^{III}$ Por, or $Fe^{III}$ Por N-oxide. He chemically synthesized each of them and characterized individually. According to his idea, for an enzyme to generate such high-valent species, a proton donor and acceptor should be located at a specified position. He introduced such residues to an appropriate position using site-directed mutagenesis technique and succeeded in converting myoglobin, an oxygen carrier protein, to a peroxidase. Thus his idea on the acid/base catalysis in the formation of high valent intermediates was proved.

## Professor Fujita

Associate Professor Makoto Fujita of Coordination Chemistry Laboratories (1997–1999; currently, Professor of Graduate School of Engineering, Nagoya University) received the Divisional Award of the Chemical Society of Japan in Organic Chemistry in 1999 for his contribution to “Precise Construction and Function of Molecular Complexes through Self-Assembly”

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

1. Development of cis-endcapped transition metals (in particular, palladium(II)) as versatile units for metal-directed self-assembly of nano-sized, discrete organic frameworks such as square molecules, linked-ring molecules (catenane), cages, tubes, and capsules.
2. Development of new functions of self-assembled hollow cage frameworks exploiting the large cavity within the cage: *e.g.*, labile (or stable) molecules are stabilized (or activated).
3. Extension of the self-assembled discrete structures into infinite systems (coordination polymers), in particular, porous coordination networks that show zeolite-like functions.

# Associate Professor Tahara's Scientific Achievements

Associate professor Tahei Tahara of Department of Vacuum UV Photoscience received the Morino Science Award in 2000 for his contribution to "Ultrafast Spectroscopic Study of the Dynamics of Condensed-Phase Molecules." Throughout his careers, he has been continuously working at the frontier of the time-resolved spectroscopic studies of photochemical processes in condensed phase. Starting from the nanosecond experiments, he has extended his research fields to even faster phenomena occurring in the picosecond and femtosecond time regions. Making the most use of vibrational and electronic spectroscopies, he has successfully clarified the dynamical properties of important elementary processes such as *cis-trans* isomerization and charge / proton transfer, which is essential for the full understanding of the chemical reactions. It is also highly noteworthy that he has been making enormous efforts to design and develop novel methods in time-resolved molecular spectroscopy. Thus, his scientific contributions have covered a broad range of subjects, and the parts of his achievements relevant to the award are summarized as follows. (1) nanosecond transient Raman study of aromatic carbonyls and charge-transfer complexes in the excited state, (2) picosecond transient Raman study of the *cis-trans* photoisomerization dynamics, and development of a picosecond two-dimensional CARS spectrometer, (3) development of a phase-stabilized femtosecond time-domain Raman spectrometer and its application to the observation of the vibrational coherence of molecular liquids, and (4) femtosecond fluorescence/absorption studies of the relaxation processes from higher excited states as well as the dynamics of photoinduced proton-transfer reactions. Recently, he has made further steps forward to extremely-fast molecular spectroscopy utilizing 10-fs pulses, and succeeded in observing the excited-state vibrational coherence.

# Associate Professor Taira's Scientific Achievements

Associate professor Takunori Taira of Laser Research Center for Molecular Science received the first research promotion award from the Miyagi Science and Technology Foundation in 2000 for his contributions to "Diode-laser-pumped microchip solid-state lasers."

Pumping of solid state active media by diodes has opened up new horizons in the solid state lasers. The professor is leading the laser society, while demonstrating new concepts such as a Nd:$YVO_4$-based microchip laser, a Q-switch-integrated frequency doubler, a Yb:YAG-based tunable green laser, and a ceramic Nd:YAG laser. All of these achievements were pioneering works and paved the way for practical compact lasers. The Nd:$YVO_4$-based microchip laser has already been launched into the market. All lasers were developed through the design rule he devised, in which he first introduced $M^2$ factor to optimize a laser cavity. The success in a Yb:YAG laser was brought about by this design rule, although the material is difficult to oscillate due to its energy structure.

He is currently expanding his research area into new laser materials such as Nd:$Y_2O_3$ and Nd:BSO, and new laser geometries like edge pumping and $\chi^{(2)}$-cascaded mode locking. His innovative ideas strongly attract researchers outside of Institute for Molecular Science, resulting in many collaborative works.