

Shigeki Kato 1949-2010



Professor Shigeki Kato passed away on March 31st, 2010 by cancer, at the age of 61. Shigeki was a pioneer in the field of chemical reaction dynamics of molecules, in both gas phase and solution. He made a wide range of original and lasting contributions to the theory of chemical reactions and dynamics, including the development of the analytic energy gradient of the multi-configuration (MC) and complete active space (CAS) self-consistent field (SCF) methods, and the construction of theoretical models in terms the intrinsic reaction coordinate (IRC) concept. He performed quantum dynamics studies of reactions in the way that the potential energy surfaces and the electronic coupling elements such as the spin-orbit interaction were both derived from high level *ab initio* electronic structure calculations. For example, his highly elaborate quantum dynamics calculations on HFCO fully explained the mode specific dissociation rates experimentally observed. Further, Shigeki developed realistic theories of chemical reaction dynamics in solution on the basis of *ab initio* electronic structure theories. He proposed the charge response kernel (CRK) method to study reaction dynamics of molecules in solution. It is unique because it was defined in terms of *ab initio* electronic structure methods. He further proposed and developed the RISM (reference interaction site model)-SCF method, which is an *ab initio* electronic structure method combined with the RISM integral equation theory for molecular liquids. This theory has an advantage in that it maintains molecular aspects of solvent and can describe local solute-solvent interactions such as hydrogen bonding. He applied it successfully to many reactions in solution to elucidate the nature and mechanism of the reactions.

Shigeki was born on March 22, 1949 in Osaka, Japan. He obtained B.S. in 1971 and Ph.D. in 1976 (under the supervision of Prof. Kenichi Fukui) both from Kyoto University. He worked with Prof. Keiji Morokuma at the Institute for Molecular Science as a Research Associate from 1977 to 1984. He moved to Nagoya University in 1984 and became Associate Professor at the University of Tokyo in 1986. Then, he came back to Kyoto University as Professor in 1990. There, he was very active not only in science but also in the administration of the university. As a result, he was elected to the Dean of the Faculty of Science, Kyoto University, for two periods, first from 2001 to 2003 and second from 2007 to 2009. He devoted himself to improve the university education and research with a firm faith. He was awarded the Japan IBM Science Prize in 1992. He was a member of the International Academy of Quantum Molecular Science since 2004 and a member of the board of Asian Pacific Association of Theoretical and Computational Chemists.