

OKAZAKI CONFERENCES

The Sixty-Fourth Okazaki Conference

Molecular Orbital Theory for the New Millennium (January 21–23, 2000)

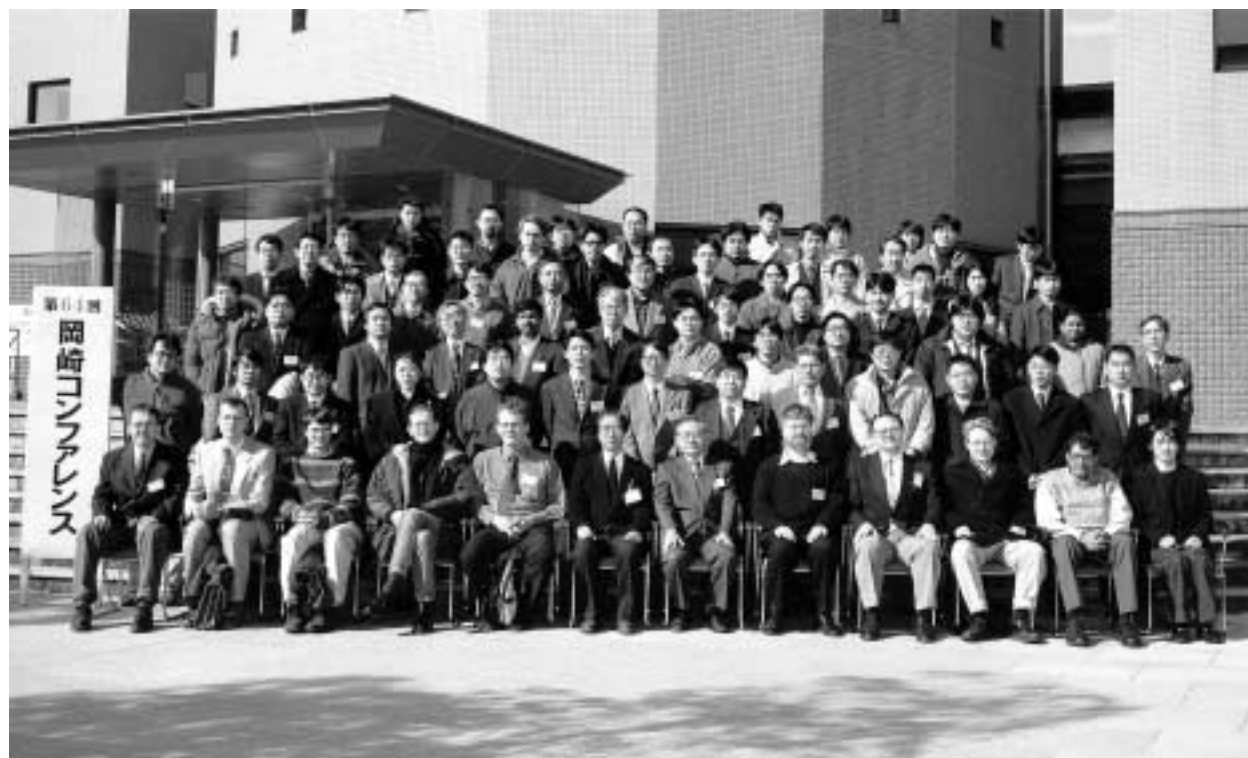
Organizers: TEN-NO, Seiichiro (*Nagoya Univ.*)
NAKANO, Haruyuki (*Univ. Tokyo*)
HADA, Masahiko (*Univ. Kyoto*)

Invited Overseas Speakers:

LINDH, Roland (*Univ. Lund, Sweden*)
HARRISON, Robert J. (*Pacific Northwest Natl. Lab., U. S. A.*)
MUKHERJEE, Debashis (*Indian Assoc. Cult. Sci., India*)
HEAD-GORDON, Marin (*Univ. California, Berkeley, U. S. A.*)
NOGA, Jozef (*Slovak Acad. Sci., Slovakia*)
KOCH, Henrik (*Univ. Southern Denmark, Odense, Denmark*)
JENSEN, Jan H. (*Univ. Iowa, USA*)
LEE, Yoon S. (*KAIST, South Korea*)
HESS, Bernd A. (*Univ. Erlangen, Germany*)

as variational parameters, 3) Multireference many electron theories for accurate calculations of quasi-degenerated systems, which may include chemical reactions and excited states, 4) Many electron theories including the complete basis set effects for calculations with spectroscopic accuracies, 5) Treatment of solvents and inert fragments as effective potentials, 6) Relativistic molecular orbital theory accurately approximating the 4-component equations. On entering the new millennium, the 64th Okazaki conference explored new dimensions and directions in the molecular orbital theory, mainly focusing on scalable quantum chemical methods and multireference many electron theories and inviting leading quantum chemists having devoted contributions for modern strategies in the molecular orbital theory.

Owing to the recent algorithmic and theoretical progresses according to the development of high-speed super computers, theoretical chemistry is entering a new dimension. For the past decade, remarkable progresses have been put forward in the molecular orbital theory especially in the following topics: 1) Scalable molecular orbital theory for large molecular systems, 2) A new molecular orbital theory using reduced density matrices



The Sixty-Fifth Okazaki Conference

Advantages of Utilization of SR in Nano-Structure Creation (January 27–29, 2000)

Organizers: URISU, Tsuneo (*IMS*)
KUROSAWA, Kou (*IMS*)

Invited Oversea Speakers:

BACHER, W. (*Forschungszentrum Karlsruhe*)
BERMUDEZ, V. M. (*Naval Res. Lab.*)
GRAY, S. M. (*Lund Univ.*)
JO, S.K. (*Kyung Won Univ.*)
SCHWENTNER, N. (*Freie Univ. Berlin*)
URQUART, S. G. (*Univ. Saskatoon*)
WEAVER, J. H. (*Univ. Illinois Urbana-Campaign*)

method of nanostructure fabrication and its evaluation technologies. Especially, the discussions were made emphasizing the role of synchrotron radiation in the nanostructure fabrication and evaluations, and the future prospects.

Nanostructures, which is expected to realize a new functional devices using quantum effects, has lately attracted considerable attention. However, techniques of fabricating the nanostructures by controlling sizes and orientations with sufficient precision are not yet sufficiently developed, and this hinders nanostructures to realize its expected excellent performances. To create ideal nanostructures, atom-molecule-level evaluation and controls of the surface reactions are essentially important, and the technological developments based on the new sciences such as synchrotron radiation science is necessary. In this conference, scientists in many different field such as surface science, solid state physics, semiconductor materials and processes, who are interested in the creation of nanostructures with controlled structures and orientations by the atom and molecule-level preciseness have gathered and discussed about the subjects of photo-excited surface reactions,

