JST Basic Research Programs

C R E S T

(Core Research for Evolutional Science and Technology)

# Annual Report for Research Work in the fiscal year 2008

**Research Area :**

**High Performance Computing for Multi-scale and Multi-physics Phenomena**

**Research Theme**

**Realizing super-accurate predictions and giant-molecular designs: breakthrough of frontiers of quantum chemistry with innovative methodologies in computational science**

**Name of Research Director, Belonging and Title:**

**Hiroshi Nakatsuji, Quantum Chemistry Research Institute, Director**

**□Note**

The content of this description is published in the HP of the Area, etc. as it is.

You are requested to take full care of the error or omission of a word, and also to prepare the report, taking the necessary security of Intellectual Property etc. into consideration.

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## §1. Outline of Research Work

Quantum principles like the Schrödinger equation govern chemistry, biology and physics of the material science. If this basic equation can be solved, we can accurately predict the phenomena of matter and science. Recently, we have discovered a general method of solving this basic equation analytically. In this project, we will apply this theory to the study of various atoms and molecules, and provide clear understanding for basic phenomena of matter and science. Our SAC/SAC-CI method is well established as a reliable method for studying ground, excited, ionized and electron attached states of diverse fields in science. In this project, this theory will be improved to be more efficient and more accurate method. Based on the SAC-CI method, new strategies will be established for investigating photo-electron processes in biological phenomena, crystals, polymers, proteins, and DNA. In this project, we will study the most of the interested phenomenon of the modern material science from small molecular to giant molecular systems seamlessly with the reliable method.

In this year, the method of the local Schrödinger equation was applied up to 6-electron atoms and molecules and very accurate physical quantities were obtained by the method. The obtained very accurate potential energy curves were confirmed the chemical reactions.

As SAC/SAC-CI science, the primal algorithm of acceleration of the SAC-CI general-R method was developed. The theory and its application program of the magnetic circular dichroism spectrum were developed based on the SAC-CI theory. In the theoretical studies of circular dichroism (CD) spectrum, the relations between sugar-basis conformation and observed spectrum were investigated for the CD spectrum of DNA. This study will initiate a new methodology to predict the helical-conformations of DNAs by theoretical calculation and spectroscopy. A systematic assignment of spectrum was provided for amino acids in the high-energy region. These results provided a fundamental aspect to study the origin of homochirality. Electronic excitation and ionization of inner-shell electron were studied and vibrational structures of spectrum were analyzed. The phosphorescence process was studied for organic electro-luminescence molecules. As application to photobiology, the color-tuning mechanism of human visual cone pigments was studied.

In quantum chemistry of giant molecular systems, the program for giant system was improved using efficient parallel computing methods. The early process of a photo-induced phase transition (PIPT) was studied. Our results suggested the possibility of concerted mechanism in PIPTs.

## §2. Content of Research Work

### (Nakatsuji Group)

### 1. Quantum chemistry as an accurate predictive science

Accurately solving the Schrödinger equation should be one of the most important central roles for quantum chemistry and the free iterative complement interaction (Free ICI) method was proposed to realize that. It has been applied to various systems and that availability and very high accuracy have