**Dear President of the Czech Academy of Sciences, Professor Eva Zažímalová,**
**Dear Honorary President of the Czech Academy of Sciences, Professor Rudolf Zahradník,**
**Dear colleagues and friends,**

Let me to introduce to you Professor Hiroshi Nakatsuji, the laureate of the Medal **„De scientia et humanitate optime meritis“**

Professor Hiroshi Nakatsuji studied in Kyoto and obtained Ph. D. in Engineering (Chemistry) in 1971.

He continued in Kyoto in 1973-1975 he spent 2 years in the US, one year with Jeremy Musher, and one year with Robert Parr. In 1990 he received professorship at the University of Kyoto.

In years 2004 to 2006 he served as director of the famous Fukui Institute for Fundamental Chemistry, currently he is director of Quantum Chemistry Research Institute and Professor Emeritus of Kyoto University. He was visiting professor in Tokyo, Nagoya and Sendai.

Professor Nakatsuji is member of International Academy of Quantum Molecular Science, where he served as General Secretary in 2012, fellow of WATOC, and other societies.

He received several prestigious awards, like Fukui Medal from Asia-Pacific Association of Theoretical and Computational Chemists, or WATOC Schrödinger Medal.

He is editor of Journal of Computational Chemistry and serves in several Advisory Editorial Boards.

## MAIN RESEARCH ACTIVITIES OF HIROSHI NAKATSUJI

As a quantum scientist, a dream of Hiroshi Nakatsuji has been to construct highly predictive and widely applicable theories and concepts that are useful in the studies of chemistry and physics. He has endeavored to make his works to be highly original, innovative, simple, intuitive, widely-applicable, and even beautiful. Further, he has tried to make up his theories starting from zero up to the useful methodologies in the fields. His main contributions are summarized as follows.

### I. Force Concept of Molecular Geometry Based on the Electrostatic (Hellmann- Feynman) Theorem.

Nakatsuji proposed a conceptual force model, called **ESF** (electrostatic force) model for molecular geometries and chemical reactions.

### II. Electronic Mechanisms and the Relativistic Effects in NMR Chemical Shifts.

NMR chemical shifts are very widely used in analytical chemistry but it is not well known that they involve a lot of information about the electronic structure of molecules. A purpose of the study of Nakatsuji is to clarify the electronic mechanisms of the metal chemical shifts and to offer the means for understanding the natures of bonding in the metal complexes.

### III. Dipped Adcluster Model (DAM) for Surface-Molecule Interactions and Reactions.

Metal surfaces show various important chemical properties, among others, the catalysis of many important reactions. When you describe surface-molecule interactions, some modeling is necessary because a surface is an

infinite system. However, the cluster model that is very often utilized as a model of a surface is very crude for a metal surface, because it cannot describe the effects of the free band electrons that are characteristic of a metal surface.

## IV. Wave Mechanics without Wave - Directly Solving the Second-Order Density Matrix without Using the Wave Function.

When the wave function of a molecule is given, we can calculate the properties of the molecule by applying the operators on the wave function. Energy and other electronic properties are such properties. Since any basic operators of properties include only one- and two-electron operators, all the properties of molecules can be calculated if the exact second-order density matrices are given. Therefore, we may construct quantum mechanics using the second-order density matrix as a basic variable instead of the wave function (**Wave Mechanics without Wave**). Nakatsuji presented in 1976 a basic equation called **density equation** (or later called "contracted" Schrödinger equation) which is equivalent to the Schrödinger equation in the space of the density-matrix. However, it took 20 years before this density equation was solved for real molecules.

## V. SAC/SAC-CI Method for Studying Chemistries of Excited and Ionized States.

Nakatsuji and Hirao proposed the SAC (symmetry adapted cluster) method for the ground states of closed and open-shell electronic structures. The SAC method is a kind of coupled cluster method that takes all the excitation operators to be symmetry adapted, so that no spin-contamination problem arises and it leads to a stable convergence to the spin-eigen function. Then,

Nakatsuji proposed in 1978 the SAC-CI (configuration interaction) method to describe accurately and efficiently the electronic structures of the excited, ionized and electron-attached states of molecules (ground and excited states of singlet to triplet spin multiplicities).

## VI. General Method of Solving the Schrödinger and Dirac-Coulomb Equations.

The Schrödinger equation and the relativistic Dirac-Coulomb equation represent the basic mathematical principles governing chemistry, biology, physics of matter, and related sciences. So, a central theoretical theme of these sciences is to establish a general method of exactly solving these two basic equations. Thereby, we can do quite accurate predictions of the phenomena without doing experiments, and therefore, this has long been a dream of theoretical chemists and physicists, though it was believed impossible by many scientists including P. Dirac, H. Eyring and others. *Recently Nakatsuji has realized this dream!* He found a general method of **analytically solving the Schrödinger equation**, breaking the "dogma" that this equation cannot be solved, which lived for over 80 years since the birth of quantum mechanics. He solved the singularity problem by introducing the scaled Schrödinger equation and opened a new field realizing the calculations of accurate analytical solutions of the Schrödinger equation for general atoms and molecules. His free iterative complement interaction (ICI) method, compactly called free complement (FC) method, combined with the variation principle gave, for example, the helium ground state energy correct up to 43 decimal figures. He further established a method to calculate the accurate analytical solutions of the Schrödinger equation without doing analytical integrations. This is a very general

methodology that is applicable to any atoms and molecules. Since the Schrödinger equation is the governing principle of chemistry, this means that chemistry will gradually change from "empirical" to "logical" science whose bases are firmly on the principles of quantum mechanics.

Hiroshi has long-term contacts with Czech science. He is professional and personal friend of many Czech theoretical chemists, like Professor Zahradník, or Professor Carsky. In 2003 I was in Boulder and during lunch break I read his first series of papers on exact solution of Schrödinger equation. The reading was much more exciting than the American lunch. I have decided to invite Hiroshi to Prague for our newly established Invited Lecture Series. Hiroshi accepted the invitation and delivered not one, but three lectures. During the dinner in Villa Lanna Professor Rudolf Zahradník suggested, that we should not stop contact with a single visit, and suggested a Japanese-Czech conference. The first one was in Prague in 2005. The second was 2 years later in Kyoto, and Hiroshi was the main organizer. Currently, the 7$^{th}$ JCS symposium is running in Prague, and Hiroshi helped tremendously the organizers with propagation and organization of the Japanese delegation.

I hope I have convinced you that Professor Nakatsuji is the excellent laureate of the top Medal of the Czech Academy of Sciences, called **„De scientia et humanitate optime meritis“,** for excellent services to science and humanity.

Thank you for your attention.