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INTRODUCTION

A Festschrift in honor of Sándor Suhai's 65th birthday

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Abstract This is a multidisciplinary multifocus issue of TCA titled the Suhai Festschrift Honorary Issue commemorating the 65th birthday of Professor Sándor Suhai and his many contributions to the fields of molecular biophysics, bioinformatics, theoretical chemistry, chemical physics and molecular biology.

1 Sándor Suhai Festschrift

1.1 Foreword by Professor Harald zur Hausen, Nobel Laureate in Physiology and Medicine

The remarkable progress of molecular biophysics, as one of the core fields in biological sciences, the quick pace of molecular modeling in unraveling DNA/RNA and protein interactions and functions, resulted in 1985 in the establishment of the Department of Molecular Biophysics at the Deutsches Krebsforschungszentrum (DKFZ, German Cancer Research Center) in Heidelberg. As the former Scientific Director of this Center who started to work in Heidelberg in 1983, I had the pleasure to install Sándor Suhai as the first head of this newly created Department in a joint appointment with the University of Heidelberg and the DKFZ. For a period of 20 years, I had the chance to follow his career and his scientific achievements.

Sándor Suhai impressed me from the beginning by his broad-based knowledge, his genuine friendliness, his prudent advice, his personal modesty, and his always helpful attitude. Within a short period of time, he established an intellectual center of biophysics at the DKFZ, attracted a number of co-workers and found increasingly national and international recognition. His team has always been

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multinational and interacted with almost every group at the Cancer Research Center. Thus, it was not too surprising that I could appoint him in 1992 as a member of the Advisory Board for the Management of the Cancer Center. He was extremely successful with applications of his group in the newly created Research Program "Genome Research and Bioinformatics", established by the German Federal Ministry of Science and Technology. In 1996, he became chairman of this national program.

I warmly congratulate Sándor Suhai to a large number of scientific achievements and I am most grateful for his years of dedicated service to the Deutsches Krebsforschungszentrum. Sándor Suhai represents a colleague of highest scientific standards, combined with personal integrity and modesty and a special sense for loyalty. I am very grateful for the years of fruitful collaboration and wish him all the best for the future.

2 Introduction

On 22 August 1944, Sándor Suhai was born in Budapest, Hungary. After his high school education, Sándor studied physics in the Institute of Solid State Physics at Eötvös Loránd University (ELTE) in Budapest, and in 1969 he received his Diploma (MSc) in Physics. From 1969 to 1975, he was a research associate in the Central Research Institute for Chemistry at the Hungarian Academy of Sciences, during which time (1972) he was awarded a PhD in theoretical physics from the University of Budapest in the Institute of Theoretical Physics. From 1975 to 1977 he was a research associate in the Institute of Theoretical Chemistry at the University of Göttingen and in 1977 he received a PhD in theoretical chemistry at the University of Erlangen-Nürnberg in the Institute of Theoretical and Physical Chemistry. From 1977 to 1983, Sándor was an Assistant Professor of Theoretical Chemistry at the University of Erlangen-Nürnberg. From 1983 to 1992, he was head of the project group "Molecular Biophysics" at the German Cancer Research Center (DKFZ) in Heidelberg, Germany. In 1984, he completed the habilitation in theoretical chemistry at the University of Erlangen-Nürnberg in the Faculty of Biology and Chemistry and in 1985 completed his habilitation in molecular bioinformatics at the University of Heidelberg in the Faculty of Theoretical Medicine. From 1992 to the present, he has been head of the Department of Molecular Biophysics at the Deutsches Krebsforschungszentrum (DKFZ). He has been professor of molecular biophysics at the University of Heidelberg, since 1993.

Upon the occasion of Professor Suhai's 65th birthday, the eight of us were inspired to organize this special focus issue of *Theoretical Chemistry Accounts* ("TCA"). For the opportunity, we are grateful to Professor Christopher J. Cramer (Chief Editor of TCA), to Ingrid Samide, Steffen Pauly, Philipp Kammerer and Petra Treiber (Springer Heidelberg, Germany) and to R. Balaji, S. A. Shine David and S. Jayagopal (Springer Mylapore, Chennai, Tamilnadu, India). In addition to former undergraduate, graduate and postdoctoral students and close collaborators of Professor Suhai, we have also invited other international researchers in the fields of molecular biophysics, biophysical chemistry, chemical physics, mathematical biology, chemistry, physics and bioinformatics to contribute to this special multidisciplinary multifocus issue of TCA. We offer here a few reflections from our own window of time with him (~1983–2009), interspersed with introductory comments on the articles in the issue.

Professor Suhai's contributions have been many to the aforementioned fields and many have been pioneering works. As you can see in Fig. 1, he got an early start in high performance supercomputing.

One of the more recent fields in which Professor Suhai has worked is the field of theoretical biospectroscopy. The use of quantum mechanics to determine the structure of biomolecules and their conformational energies is but one small application. In many cases, one can in addition use classical mechanics force fields to get the same information. Indeed quantum mechanical calculations have been combined with experimental data to parameterize a majority of the currently used molecular mechanics force

Fig. 1 Little Sándor with his first computational efforts

fields. Where classical mechanics is not useful is in enzymatic reactions involving bond breaking and in predicting, interpreting and understanding the electronic absorption (EA), electronic circular dichroism (ECD), fluorescence, vibrational circular dichroism (VCD) and Raman optical activity (ROA) spectra in a variety of diverse biological environments. The interaction of radiation with matter (biological molecules, complexes and life itself) is fundamental to life processes, and it must be treated quantum mechanically. The review and overview articles by Kukushkin/Jalkanen, Petersen/Bohr and March/Matthai deal with many of the aspects of quantum mechanics which are important in molecular biophysics, molecular biology and molecular medicine.

In the group of Professor Suhai, pioneering work on the treatment of the aqueous environment in determining the species and conformers present in aqueous solution have been undertaken. In work by Han, Jalkanen, Elstner and Suhai an example was provided wherein the spectrally active species of interest was not the individual solute molecule, but the hydrated/solvated species, in this case the alanine dipeptide, *N*-acetyl L-alanine *N*′-methylamide (NALANMA). The conformer of NALANMA found in aqueous solution is not even a stable minimum on the gas-phase/isolated state potential energy surface. Hence, explicit water molecules must be included in molecular simulations of NALNMA and many other biomolecules. The use of continuum solvent models alone has not been able to even determine the correct structure. This has changed the paradigm for modeling and interpreting the spectroscopic data of amino acids and peptides in aqueous solution.

Professor Suhai was one of the first scientists to recognize the importance that density functional methods (DFT) were going to have in the study of biological molecules. With his student Martina Kieninger, he embarked on a research line to modify existent DFT codes (deMon) and to apply DFT methods to small molecules as prototypes of the problems to be faced in biological systems. Seminal papers were published jointly on the resistance to rotation of protein backbones and on the ability of the then contemporary methods to address hydrogen bonding. The collaboration extended to other areas such as antisense DNA or thermochemical calculations and continued well after Dr. Kieninger moved to a new position with Professor Oscar N. Ventura at the University of Uruguay, where she still works.

The modeling of larger and larger biological molecules has, of course, required simplifying assumptions and approximations. In collaboration with Professor Thomas Frauenheim's laboratory, Marcus Elstner, Thomas Niehaus, Kenneth Frimand, Michaela Knapp-Mohammady, Henrik G. Bohr, Emad Tajkhorshid, Nicoleta Bondar, Wenge Han, Karl J. Jalkanen and others have developed and tested a semi-empirical density functional theory-based method, the so-called self-consistent charge (SCC) density functional tight binding (SCC-DFTB) method and its extension to include dispersion forces, SCC-DFTB + Dispersion. In addition to its use in optimizing geometries, determining conformational energies and use in molecular dynamics simulations, it has also been used for determining the vibrational frequencies of biomolecules, and when combined with accurate atomic polar tensors (APTs) and atomic axial tensors (AATs), vibrational absorption (VA) and vibrational circular dichroism (VCD) intensities. The ability to reproduce the VA and VCD intensities is a very tough test for the accuracy of a molecular mechanics force field, semi-empirical methods, or ab initio or DFT methods. The SCC-DFTB method has now largely replaced the earlier developed AM1 and PM3 semi-empirical wave function-based methods. The PM6 method of J. Stewart and the recently developed methods of W. Thiel are also more accurate than the older AM1 and PM3 methods. These are but two of the major developments that have been undertaken in large part in the laboratories of Professor Suhai and his collaborators.

In the field of quantum chemistry for polymers, Professor Suhai had a chance to collaborate with Prof. Akira Imamura, while Sándor was an Assistant Professor in Professor János Ladik's laboratory at the University of Erlangen-Nürnberg. In this collaboration, a quantum chemical approach to aperiodic polymers was developed based on Prof. Suhai's ab initio program, which had been incorporated into Gaussian 70 for polymer calculations under a periodic-boundary condition. After that, Professor Akira Imamura was invited several times by Prof. Suhai to the DKFZ, and got the idea of an elongation method for efficient computation of random polymers/biopolymers. In 1988, Prof. Yuriko Aoki (who was a student of Prof. Imamura's at Hiroshima University) had a chance to stay in Professor Suhai's group at DKFZ as an Alexander von Humboldt fellow to develop this idea at the DFT level. Through the collaboration on late 1990s, several treatments for periodic and aperiodic polymers were developed at the level of semi-empirical and ab initio MO methods and tested on simple systems as the first step toward gigantic systems. This project continues to further develop to Hartree–Fock and post-Hartree–Fock levels for biopolymers as proteins/DNA (and more general applications to two- and three- dimensional systems) at Kyushu University.

Many of these and other fields are represented by articles in this Festschrift by former students, postdocs and collaborators.

Beyond molecular biophysics, developments in bioinformatics and genome research added a completely new research field to Prof. Suhai′s activities in the years 1983–

1984. Together with Prof. zur Hausen, they early realized the importance of mathematical and information theoretical methods in modern molecular biology. DKFZ pioneered this field by founding one of the first theoretical bioinformatics groups in Europe and, with the substantial financial support of the European Union, Prof. Suhai implemented the European Data Resource for Human Genome Research in Heidelberg in 1986. DKFZ remained one of the leading German research institutions in bioinformatics for about two decades and Prof. Suhai coordinated several national research programs in the field funded by the Federal Ministry of Research and Technology. He also served as a head of the German node in the European Molecular Biology Network (EMBNet) for about 15 years. Besides bioinformatics, genome research in general became an integral part of cancer research in Heidelberg. Prof. Suhai was appointed as the first Coordinator of the intramural Program in Genome Research and Bioinformatics at DKFZ in 1992.

For a period of 17 years, Professor Sándor Suhai was the Head of the Department of Molecular Biophysics at the German Cancer Research Center.

One of his main characteristics as a leader was that he always gave his employees a high amount of scientific freedom and autonomy. His highly skilled and literate mind made him a great visionary, competent and expert in all fields that he had to deal with.

From the point of view of his co-workers, he was an outstanding boss who brought his group a remarkable reputation in the international scientific community. He attracted countless guest scientists, post-graduate and graduate students from all over the world to his group. To all of these multinational co-workers, he was open minded, providing a good atmosphere that allowed the team to work efficiently and with congeniality.

The most astonishing aspect to most people when they joined the group was the lack of hierarchy; independent of the status of the employees, he was just 'Alex' to everybody.

The reputation of his department was so high that all members of his staff got the best possibilities for their future scientific research and career. During the time of working in his group, innumerable genuine and long-standing personal bonds arose that will always play an important role in the future life of all members.

Figures 1 and 2 show Professor Suhai in an early and a later phase of his computational studies. Figure 3 shows him at the PhD defence of a former co-worker in his group who, after receiving much encouragement from "Alex" and other co-workers and colleagues at the DKFZ in Heidelberg, decided to further his education and obtained a PhD in the field of molecular biophysics in Professor Risto M. Nieminen's Laboratory of Physics at Helsinki University of Technology in Espoo, Finland. Figure 4 presents the status of the Molecular Biophysics group in 1994.

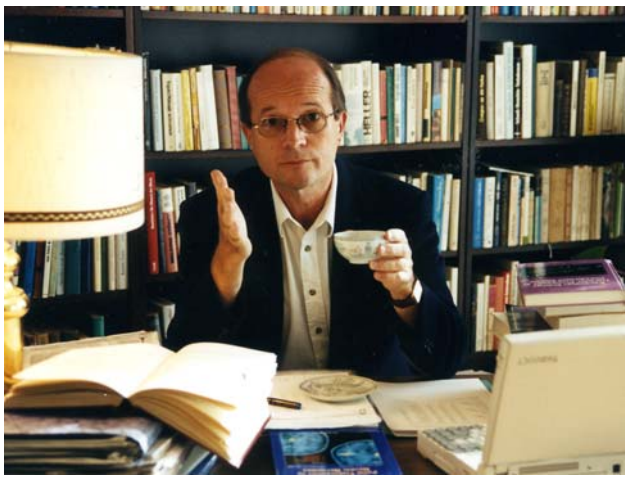

Fig. 2 Sándor at a further stage, in the middle of his scientific life

Fig. 3 PhD defense of Ivan M. Degtyarenko (from left to right): Carme Rovira, Sándor Suhai, Ivan M. Degtyarenko, Karl J. Jalkanen and Risto M. Nieminen

Fig. 4 Department of Molecular Biophysics Picture from 1994

We are grateful to the many authors who decided to submit their manuscripts for publication in this special focus issue of TCA and the many anonymous referees who have taken their valuable time to provide invaluable recommendations and evaluations of the original submissions and subsequent revisions. The diversity and breadth of the topics covered by manuscripts matches closely the diversity and breadth of the many fields in which Professor Suhai and his group have worked; starting from fundamental developments in both molecular biophysics and chemical physics (J. Schirmer, A. Vibok, B. Champagne, P. Carbonniere, E.K.U. Gross, K. Kneipp, I. Grabowski, J. Bohr, A. Dreuw, J. Pipek, A. Bende, Y. Aoki, A.K. Kukushkin, K.J. Jalkanen, J. Ladik, T.A. Niehaus, L. Noodleman, W. Han, I. Mayer, D.F. McIntosh, M.S. Gordon and G.J. Kearley), to applications of both quantum and classical mechanics to solve fundamental problems in molecular biophysics and molecular biology (P.C. Mishra, C.C. Matthai, J. Langowski, N. Bondar, M. Elstner, H.G. Bohr, A.H. deVries, E. Tajkhorshid, A. Der, C.F. Guerra, M. Zacharias, T. van Mourik, V.I. Danilov, B. Paizs, M. Knapp-Mohammady, N.H. March, M. Kieninger, O.N. Ventura, and A.K. Bronowska), to developments and applications in bioinformatics (B. Mirkin, C. de Val, A. Hotz-Wagenblatt, K.-H. Glatting, A. Hatzigeorgiou, M. Reczko, C. Verma, P. Zielenkiewicz, A. Vinayagam and S. Kogenaru), to scientific visualization and publishing (V. Vasilyev), to the biophysics/biomathematics of drug delivery (X. Lou), and finally to breast cancer detection (A.A. Martin).