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INTRODUCTION

A Festschrift in honor of Akira Imamura's 77th birthday, his recent retirement, and his many contributions to theoretical chemistry

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Abstract The Imamura Festschrift Issue of Theoretical Chemistry Accounts is a special multifocus international issue commemorating the 77th birthday of Professor Akira Imamura and his many contributions to the fields of theoretical chemistry, polymer science, molecular biophysics, chemical physics, and molecular biology. This issue has contributions in theoretical developments of methods applicable to larger polymeric systems, for example, the elongation method pioneered by Professor Imamura and his group, and more recently by the groups of Professor Yuriko Aoki at Kyushu University and Professor Feng Long Gu at South China Normal University, supported by several funds from the Japan Science and Technology Agency (JST). In addition, there are contributions from top experimental and theoretical groups in the areas of nanotechnology, bionanotechnology, quantum transport theory, molecular biophysics, molecular electronics, and even molecular medicine and medical diagnostics, where the marriage between theory and experiment is very important to be able to fully understand, interpret, and utilize the wealth of new and exciting experimental data. The development of new and refined methods, and the extension of older more conventional methods, will be required for these fields to continue to evolve/co-evolve and develop, as they have in the last 60 years. But to evolve in a guided fashion (guided evolution), that is, to meet the needs and functions of not only the individual scientists and research groups but also of society in general, will require a concerted effort from not only experimentalists and theoreticians in each individual subdiscipline but also for them to work together and share their accumulated knowledge and experience, as is now being done in various research networks around the world, including the one originally initiated/formed by Professor Imamura and Professor Janos Ladik at the Third International Congress of Quantum Chemistry (ICQC) in Kyoto, Japan. Through this network, Professor Imamura has been able to pass on a wealth of knowledge, expertise, and experience to the current and future generations of scientists in Germany, the United States, and China, as Professor Imamura is still doing with his lectures both in Japan at Kyushu University and in China at South China Normal University, and previously in Erlangen at the University of Erlangen, in Heidelberg at the German Cancer Research Center (DKFZ) in Germany, and in Ithaca, New York at Cornell University in the United States. He has been a real example of the modern protean research scientist and

Dedicated to Professor Akira Imamura on the occasion of his 77th birthday and published as part of the Imamura Festschrift Issue.

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professor who has continued to be in research and teaching, active well beyond the formerly set retirement age of 63 or 65 set by society. The idea that researchers and professors cannot be active in their 60s, 70s, and 80s has now also been shown to be a misconception that needs to be corrected at the funding and institutional levels. Too many very active, knowledgeable, and experienced researchers and professors have been forced to stand on the sidelines, while those who have replaced them have very little practical knowledge, expertise, and more importantly, life experience. A whole generation of young academics are being hired who have never worked a day in industry, never visited an industrial laboratory and/or research group, and hence are unable, (don't know) and in many cases, unwilling to train and educate their students with the skills they need to not only work in industry but also to create new and exciting new industries. The idea that the large chemical and pharmaceutical companies and government laboartories will hire all of the ever increasing numbers of undergraduate and graduate (MSc and PhD) students no longer applies. The university mission is no longer just to teach, give knowledge, and to do research, but also to innovate, that is, to train the students to take their acquired knowledge from their text books and apply it with the newly acquired knowledge in the research laboratories to start and develop new industries and companies. But this means that the students need to be trained in the fields of engineering economics, finance, and scientific and international law, so that they are able to undertake such projects, in addition to understanding and applying their scientific knowledge. It will also require a concerted effort by funding agencies, state, local, federal, and even international bodies that seek to create and sustain strong economies and infrastructure, which will support and be supported by the highly motivated, trained, and educated work forces. The third pillar is now being established, but it needs to now be totally and completely integrated with the other establishments and infrastructure.

Keywords Elongation method · Raman spectroscopy · Collagen · Electronic exited states · Quantum transport theory · Vertically aligned carbon nanotubes · Coordination chemistry · Nonlinear optical properties · Zeolites · Medical diagnostics · Relativistic effects · Retinal protein · Thiacrown metal complexes · Long-range corrected density functional theory · Local response dispersion corrected density functional theory

1 Introduction

From Professor Yuriko Aoki, the co-organizer of the Imamura Festschrift Issue of TCA, former PhD student and many year collaborator of Professor Akira Imamura, and now Professor of Material Sciences at Kyushu University:

We would like to commemorate the 77th birthday "Kijyu" of Professor Akira Imamura on August 15, 2011 with this special issue of TCA. Since I first started learning the basics of quantum chemistry from him when I was a graduate student, I have continued to take the serious attitude that he has instilled in me towards academic research for nearly 30 years. Not only did I receive a theoretical foundation in quantum chemistry from him but I also learned how to conduct/undertake research and how to value the importance of new ideas and originality in research. These characteristics have very greatly influenced my subsequent research life, though, unfortunately, my flowers have still not completely opened/blossomed, and I still have much yet to do and to learn.

Thirteen years has already passed, since he retired as Professor of Physical Chemistry from Hiroshima University. Yet, in the first 13 years of his retirement from science, he has been devoted to educational, teaching, instructional, and administrational issues at Hiroshima Kokusai Gakuin University. In addition, he has personally been able to continue doing basic research, for which we have reverence and great respect. And even now, he is energetically giving lectures to students in quantum chemistry both here in Japan at Kyushu University in Kasuga, Fukuoka, and also at South China Normal University in Guangzhou, Guangdong, China. We have no doubt that he will have a great influence on our young students with his very kind and thorough teaching as well. We are very pleased to be able to contribute to the research articles from our group, which will be published in the Imamura Festschrift Issue of Theoretical Chemistry Accounts in honor of Professor Imamura achievements to date. It has been now 20 years, since he proposed the elongation method in 1991 [1]. Thus, at Kyushu University, we now can conduct research based on elongation method owing to his very simple and very interesting idea—Theoretical Synthesis of Random Polymers (elongation method), and our thanks to him will never end. We hope that we have completed the elongation software as widely recognized in the world at latest before "Beiju" (88 years old). We pray sincerely that he will spend forever on enjoyable research life with good health, while being issued a new idea.

2 Professor Akira Imamura

Professor Imamura has been a pioneering researcher in the development and application of quantum mechanical methods for large systems. Initially, he developed semi-empirical methods for analysis of organic molecule and large bio-systems and extended them in collaboration with other Japanese, American, and European scientists,

especially in molecular biophysics field, subsequently extended these methods to the Hartree–Fock level, and more recently, extended them to post Hartree–Fock methods. A more recent application has also been to extend and apply quantum-based methods to π-conjugated conducting polymer, transport phenomena with quantum molecular wires, and spin-based molecular devices.

3 Brief curriculum vitae

3.1 Professor Akira Imamura

Born: 15 August 1934, Shiga Prefecture, Japan
1957, Graduated in Chemistry from B. C. Kyoto University, Japan
1959, Graduated in Chemistry from M. C. Kyoto University, Japan
1962, Graduated in Chemistry from D. C. Kyoto University, Japan (Dept. of Fuel Chemistry, Faculty of Engineering); 1963, Ph.D. in Chemistry by Supervisor Prof. **Kenichi Fukui**
1962, Nippon Telegram & Telephone Public Corporation, Research Associate at Electrical Communication Laboratory
1964, Head of the section of Quantum Chemistry, Division of Biophysics, National Cancer Center Research Institute, Japan
1966–1967, Research Associate, Dept. of Chem. Cornell University (In the laboratory of Prof. **Roald Hoffmann**)
1975, Professor of Chemistry, Shiga University of Medical Science
1981, Guest Professor, Erlangen Universität at Institut für Theoretische Chemie (In the laboratory of Prof. **János Ladik**)
1982, Professor of Physical Chemistry, Hiroshima University, Dept. of Chemistry, Faculty of Science
1988–1989, Visiting Professor of Institute for Molecular Science (IMS), Okazaki, Japan
1991–1994, Japan Science and Technology Agency (JST)-PRESTO researcher
1998, Retired Hiroshima University, Dept. of Chemistry, Faculty of Science
1998, Visiting Researcher, Deutsches Krebsforschungszentrum, Molekulare Biophysik (In the laboratory of Prof. **Sándor Suhai**)
1999, Professor of Mathematics, Faculty of Engineering, Hiroshima Kokusai Gakuin University
2001, Dean of the Faculty of Engineering, Hiroshima Kokusai Gakuin University
2005, President of Hiroshima Kokusai Gakuin University
2010, Retired Hiroshima Kokusai Gakuin University

4 Significant three papers

1. Benzynes, Dehydroconjugated Molecules, and the Interaction of Orbitals Separated by a Number of Intervening σ Bonds.
   R. Hoffmann, A. Imamura, and W. J. Hehre, *J. Am. Chem. Soc.*, **90**, 1499–1509 (1968).
   - Pioneering paper of Hoffmann, Imamura, and Hehre (HIH) on through-space (TS)/ through-bond (TB) interaction concept. It has been cited over 800 times and selected as Theoretical Chemistry Accounts New Century Issue with perspective by K. D. Jordan, Theor Chem Acc (2000) 103:286–288 as one of 66 significant articles in 20th century's theoretical chemistry).
2. Electronic Structures of Polymers Using the Tight-Binding Approximation. I. Polyethylene by the Extended Hückel Method.
   A. Imamura, *J. Chem. Phys.*, **52**, 3168–3175 (1970).
   - Screw Axis Symmetry under periodic boundary condition was firstly introduced into periodic polymer systems including both π and σ orbitals.
3. A Theoretical Synthesis of Polymers by Using Uniform Localization of Molecular Orbitals: Proposal of an Elongation Method.
   A. Imamura, Y. Aoki, and K. Maekawa, *J. Chem. Phys.*, **95**, 5419–5431 (1991).
   - Development of Efficient and accurate quantum chemistry calculations for random polymers: PRESTO (Precursory Research for Embryonic Science and Technology) fund was awarded by Japan Science and Technology Agency (JST), 1991.

Professor Akira Imamura-sensei in the current stage of his scientific career in Japan.

5 Corresponding authors of contributions

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1. Imamura A, Aoki Y, Maekawa K (1991) A theoretical synthesis of polymers using uniform localization of molecular orbitals: proposal of an elongation method. J Chem Phys 95:5419–5431