Theor Chem Acc (2011) 130:575–593
DOI 10.1007/s00214-011-0988-7

OVERVIEW

# Akira Imamura: a scientific memoir (1950–2011)

**Akira Imamura**

## 1 My senior high school days

I entered Otsu Senior High School in Otsu City in the Shiga prefecture in 1950 and graduated from Otsu Higashi (East in English) Senior High School in 1953. However, I didn't move from one high school to another. I entered and graduated from the same high school, but the name had changed. This was due to the violent change in the educational system in Japan after World War II. This was intimately connected to the sudden change in the morality and political system in Japan at that time. This turning point in the history of Japan made me certain that I should be very flexible in everything that I did and would do in life, and that there are not absolute justices and truths, but relative ones. One needs to have a reference frame in which to measure things and oneself. One is very much influenced by one's surroundings, just like atoms and molecules. This way of thinking has had a very important effect and influence on my thought processes and has affected and influenced my various research projects and endeavors. I was fortunate to get a very good education and foundation at Otsu Higashi Senior High School which prepared me for the next stage of my education, career and life development.

## 2 Kyoto University

In 1953, I entered the Department of Fuel Chemistry in the Faculty of Engineering at Kyoto University because Otsu City is located near Kyoto City, and I had graduated from high school in Ostu City. Many of the students like I who chose to study in the Faculty of Engineering at Kyoto University believed that they would have great chances and opportunities to get good industrial jobs after graduation, and to be able to help rebuild Japanese industry, which had been devastated by the long war.

Already as an undergraduate student I attended special departmental meetings/seminars in which the faculty members and students got together and the full professors gave us understandable talks about the current content and aspects of their ongoing active research projects. Among those who gave very interesting and thought provoking seminars was Professor Kenichi Fukui, who in 1981 would be awarded the Nobel Prize in chemistry. He spoke about the essence of frontier electron theory and its applications for predicting and understanding chemical structures and reactivity. His short speech had a strong impact on me. From that moment on, I decided to change my plan to pursue a job in industry to pursue one in academics (fundamental research). I would pursue an academic career which would allow me to do basic research instead of going to work in industry and apply, and perhaps perfect and extend the knowledge already known. My destiny had been set by attending an undergraduate seminar at a research intensive Japanese university, which Kyoto University always has been. From that day on, I would start my journey on one of the many possible paths which would ultimately lead to a tenured academic position at a research intensive university in Japan. Such a career path would not be (and today is not) as easy as I or anyone else would have

A. Imamura (✉)
Hiroshima Kokusai Gakuin University,
6-20-1 Nakano, Aki-ku, Hiroshima 739-0321, Japan
e-mail: a.imamura@waltz.ocn.ne.jp

A. Imamura
Department of Energy and Material Sciences,
Kyushu University, 6-1 Kasugakoen, Kasuga,
Fukuoka 816-8580, Japan

expected. A career as a research-intensive academic research professor is a never ending one. The search and quest for knowledge and understanding never ends, as I would soon find out. There is always something more to learn, to discover, to find out, and then to teach one's young undergraduate students, and a bit older graduate and postdoctoral students. Nature has many hidden treasures and wonders which are there for us to uncover and find, if we only have the patience, diligence and willingness to be able to spend the time and make the effort and sacrifices required to do what it takes.

I entered the research laboratory of Prof. Fukui as a fourth-year undergraduate student, and was admitted in 1957 into the Masters Degree Program in the Graduate School at Kyoto University and was initially attached to the ***Fukui Laboratory***. The first research project offered to me by Prof. Fukui was to work on further developing a theoretical approach to treat aromaticity in connection with the so-called 4n + 2 ($\pi$ electron) rule. By using perturbation theory, we succeeded in relating the stability of aromatic hydrocarbons with 4n + 2 $\pi$ electron ring structure formation [1]. In 1959, I was accepted into the Doctoral (PhD) Degree Program and my initial research project in the Fukui Laboratory involved using molecular orbital methods to study charge transfer complexes, the subject of which had been suggested by Associate Prof. Yonezawa who was collaborating with Prof. Fukui to develop frontier electron theory. The theory of charge transfer complexes had already been developed by Prof. R. S. Mulliken in 1952 [2], in which the charge transfer interaction was incorporated in terms of the highest occupied molecular orbital (HOMO) of the electron donor and the lowest occupied molecular orbital (LUMO) of the electron acceptor. One of the important aspects of this theory was the concept of the coincidence of the symmetry of the HOMO and the LUMO for an effective charge transfer interaction to be possible and to be present. I applied perturbation theory to the charge transfer interaction and derived a formula similar to the superdelocalizability formula in frontier electron theory.

To be more specific, the numerator in the formula is $(\mathrm{Cir} + \mathrm{Cis})^2$ instead of $(\mathrm{Cir}^2 + \mathrm{Cis}^2)$ for the two-center interaction [3]. This form of the numerator implies that the symmetry of molecular orbitals plays an important role in the charge transfer interaction. Moreover, this formula includes the contributions from not only the HOMO and the LUMO, but also all other orbitals in an analogous way to that given in the frontier electron theory. It is noteworthy that this formula can be considered as a possible motivating factor for the development of Woodward–Hoffmann theory and the so-called Woodward–Hoffman frontier orbital rules. In fact, Prof. Fukui applied this formula to the Diels–Alder reaction and indicated that the symmetry of the molecular orbitals play an essential role in the chemical reaction in 1964 [4], one year prior to the publication of Woodward–Hoffmann theory [5–7].

Moreover, I tried to apply the theory of charge transfer complexes to the organic semiconductor which had been experimentally discovered and developed by Akamatsu and Inokuchi, but I didn't write up my work and submit it for publication. I also calculated the electronic structure of various biologically interesting carcinogenic compounds in collaboration with Dr. Nagata who was a research associate in Fukui's laboratory. These investigations were part of my PhD work in the Fukui laboratory at Kyoto University. The problem of accurately predicting the relative energies of charge transfer states, especially those involving charge transfer from one orbital to another in the same molecule (intramolecular charge transfer) or to an orbital on other molecule (intermolecular charge transfer) is still an active field for research in 2011. Fluorescence or Förster resonance energy transfer (FRET) in many cases involves charge transfer after the initial absorption of a visible photon of light. In organic semiconductors, a field of active research today, it is important that one have a theory which not only is able to reproduce the ground electronic state and its electronic and magnetic properties, but also those of the various low lying (accessible) electronic states. The work undertaken during my PhD-years would prepare me for work in this exciting and still active research area. The methods at the time, both in condensed matter physics, density functional theory and tight-binding models, were not really adequate to treat organic semiconductors, as they had been developed to treat solid state physics systems. It would be years before density functional theory and the tight-binding approximate models would be able to treat these systems with chemical accuracy.

In 1963, I received my PhD in chemistry from Kyoto University with Prof. Kenichi Fukui as my PhD supervisor (Doktorvater in German). During the period of 1962–1964, I worked as a research associate in the electrical communication laboratory of Nippon Telegraph and Telephone Public Corporation (now NTT, Inc.) and engaged in experimental studies on the physico-chemical properties of organic semiconductors such as polytetracyanoethylene copper chelate films.

## 3 National Cancer Center Research Institute, Tokyo

In May of 1964, Dr. Chikayoshi Nagata who had been a research associate in Fukui's laboratory of Kyoto University and was the Chief of the Division of the Biophysics at that time, kindly gave me the opportunity to become the Head of the Quantum Chemistry Section in the Division of Biophysics at the National Cancer Center Research Institute

(NCCRI) of Japan. From that time on, I began to try to determine the relationships between electronic structure of various carcinogenic compounds and their carcinogenic activities. As was to be expected, it was very difficult to find the direct functional relationships due to the intricacy of the networks of coupled biochemical reactions in living systems. The initial reactions that carcinogenic compounds would induce in living systems were thought to be few, while carcinogenicity was thought to be the final result of many different biochemical reactions and processes which would be influenced by the initial event. In many instances, cancer results decades after the initial exposure to some chemical, radiation, foreign organism, or combination of the three. A chain of events is started which ultimately leads to cancer, and one needs to figure out how to stop this chain of events if one cannot prevent it from initially occurring. Cancer was then and still is one of the most difficult of diseases to determine the initial cause and then to stop or cure.

During this time at the NCCRI, I started to develop a methodology for a semiempirical molecular orbital theory which included both $\sigma$ and $\pi$ electrons, hoping to extend the $\pi$ electron theory of Hückel. However, I discontinued my research into the development of a semiempirical $\sigma$ and $\pi$ electron molecular orbital theory with the publication of the excellent and beautiful works of J. A. Pople, D. P. Santry and G. A. Segal based on the complete neglect of differential overlap, the so-called CNDO method [8, 9]. What I was attempting to develop had been developed by these three researchers at the Carnegie Institute of Technology and Mellon Institute of Industrial Research (which merged in 1967 to become Carnegie Mellon University) in the USA. John A. Pople would later go on to win the Nobel Prize in Chemistry for this and his subsequent work in quantum chemistry. I had chosen the right project to work on, but was beat to the punch by John and his two protégées.

## 4 Cornell University, Ithaca

In 1966, I was allowed to take a leave of absence from the National Cancer Center Research Institute in Tokyo and spend a ***sabbatical*** period in the laboratory of Prof. Roald Hoffmann at Cornell University in Ithaca, New York. From August of 1966 until December of 1967, I was engaged in various collaborative research projects with Prof. Hoffmann. One project was to work on the theoretical development of the now famous through-space versus through-bond interactions in collaboration with Prof. Hoffmann. I developed these concepts mathematically by applying perturbation theory and the result was a beautiful and elegant explanation of the mathematical equations in terms of through-space/through-bond interactions by Hoffmann [10]. Another interesting project was our study of the relationship between the molecular and electronic structures of biphenyl, fulvalene and their analogs in the ground and excited electronic states. At the time, it was experimentally known that biphenyl had a twisted ground electronic state structure and a planar first excited electronic state structure. I could provide an explanation and understanding of these experimental results based on molecular orbital theory, that is, I succeeded to explain this experimental result by the combination of steric effects between the hydrogen atoms bonded to the phenyl rings and $\pi$ electron conjugation between the phenyl rings governed by the symmetry of the occupied molecular orbitals in the ground and excited electronic states. Here, we showed that by analyzing the electronic structure of orbitals occupied in the various electronic states, one could predict the geometrical structure. One of the keys to relating quantum chemical calculations to geometrical structure had been found. The next one was of course reactivity, that is, how the orbitals on two different molecules could be used to predict how the molecules would react, and the end products.

The molecular orbital analysis method we used to explain the ground and excited electronic structures and hence geometries for the neutral species can also be applied to explain and predict the molecular structures for both the cationic and anionic species of these molecules in the ground and excited states although we hadn't stated this specifically in our publication [11]. We also developed a general perturbation theory for extended Hückel theory which includes perturbed Coulomb and resonance integrals as well as overlap integral terms [12]. Prof. Hoffmann asked me to use the extended Hückel molecular orbital method to perform a conformational analysis for various dipeptides including *N*-acetyl-*N*'-methyl-glycylamide [13]. The conformational maps which resulted from our investigation were very similar to the ones which were derived by Prof. Scheraga's group in Cornell using empirically derived Lennard–Jones potential energy functions between atoms (so-called Ramachandran plots for each amino acid residue). Our conformational maps were thought to be more reliable and to provide more chemical and physical insight and understanding, as our approach was based on molecular orbital theory and included many of the interactions which are missing when one uses a simple Lennard–Jones potential energy function. The seeds for more work in this area by me and my group in Japan were sown during my sabbatical stay in the Hoffmann's laboratory at Cornell during the 1 year and 4 months I was in Ithaca.

The sabbatical experience gave me many useful results and fruitful ideas which I would use and be able to draw on during my research career. In addition, I was able to gain a general view of Japan and Japanese science from outside of Japan, something which is good for every citizen of every country to get. One's perspective of oneself, one's country, and one's culture and one's way of doing science change or at least are seen under a different light when one is viewing them from the outside, rather than from within. I also have to mention that my many talks and discussions with Prof. Hoffmann were very stimulating, thought provoking, and instructive. Included among them was the thought that ONE of the aims of theoretical research should be to provide the guiding principles for organic and inorganic experimental chemists to use in the design of their future experiments. And certainly, the concept of through-space versus through-bond interactions is one of the most important. Indeed, this is still an active area of research over 50 years later.

## 5 National Cancer Center Research Institute, Tokyo *again*

After returning to Japan, I initiated a series of molecular orbital research projects to investigate various polymers utilizing the tight-binding approximation from solid state physics which I had studied when I had been a student in Prof. Fukui's laboratory of Kyoto University. I first applied a tight-binding method to investigate various conformations of polyethylene in the framework of extended Hückel theory. In order to be able to perform such calculations for polyethylene in various screw axis symmetries, I had to perform a unitary transformation of the $x$- and $y$-coordinate axes of the atomic orbital basis set in order to be consistent with the screw axis symmetry.

To the best of my knowledge, I was the first one in the world to develop and test an approach to treat polymeric systems with various screw symmetries using molecular orbital-based methodology, the method described in the first of a series of papers [14]. The second paper of this series was to apply this newly developed approach to study polyethylene and polyglycine using the CNDO/2 method in collaboration with Ms. Fujita [15]. We found that our approach was additionally applicable in the framework of self-consistent field (SCF) methods, although we did experience some problems with convergence. We experienced some divergent behavior during the SCF procedure for certain systems, especially in the case where the hydrogen bonds were interacting with each other as in α-helices. In order to overcome the divergence problems, I developed a novel iterative procedure that I implemented in the SCF method I was using for polymers by using the density matrix which had been originally formulated by McWeeny [16].

Moreover, I applied this procedure to investigate polyglycine and poly-L-alanine in the planar, the right-handed α-helix and the left-handed α-helix conformations [17]. The calculated relative stabilities of the three conformations for poly-L-alanine was the right-handed > left-handed > planar, which is in agreement with the experimental results. The reason why the right-handed α-helix is more stable than left-handed α-helix was scrutinized by partitioning the total energy into the partial contributions of fragments of the polymer. Here, we found that the difference in the interaction energy between methyl group and remote carbonyl group is responsible for the stability of the right-handed α-helix. It should be stressed that this interaction between methyl and carbonyl groups could be regarded as a kind of hydrogen bond. After publishing these results, I was invited to give lectures at many physics meetings and in addition, at many biochemistry meetings.

I was quite surprised since the responses to my results were completely different by the two communities. That is, the physics community was in general surprised by the complexity of the system in comparison with other molecules containing a few atoms. On the other hand, the community of biochemists took not much notice of the computed system because of its simplicity in comparison with the real life biopolymers in cells. They pointed out strongly that the electronic structures of periodic polypeptides were of little practical use since the biological function of most proteins was intimately related to its aperiodicity. What was also remarked by Kendrew and others after the publication of the first crystal structure of a protein was that there was very little symmetry. Condensed matter and solid state physicists who had developed the tight-binding method were used to treating periodic systems, crystalline solids and not amorphous non-crystalline glasses. After my discussions with the biochemistry community, I fully recognized and appreciated the need for the development of computational methods for non-periodic polymers would be indispensable for quantum chemistry methods to be able to contribute to biochemical problems where symmetry was to a large extent lacking.

In parallel with this research project, I was developing a method to predict the catalytic activity in connection with orbital mixings with Prof. Hirano at the University of Tokyo. He pointed out to me the interesting paper written by Houk and coworkers, in which the change in the regioselectivity of Lewis acid catalysis was explained by the changes in the HOMOs and LUMOs obtained using the semiempirical CNDO/2 molecular orbital theory. However, no theoretical basis for the changes in the HOMOs and LUMOs had been given [18]. Therefore, we analyzed the changes in all of the molecular orbitals in terms of the interactions induced during Lewis acid catalysis in terms of perturbation theory [19].

As a result of this analysis, it was shown that orbital mixings were responsible for the changes in the molecular orbitals involved in catalysis, including the HOMOs and LUMOs. Furthermore, there had been two factors which control the magnitude of the orbital mixings; one is the perturbation due to electrostatic interaction and the other due to the overlap of the orbitals. The former were designated as static orbital mixing and the latter as dynamic orbital mixing. General rules were derived to predict the magnitude of the orbital mixings. These rules were successfully applied to Lewis acid catalyzed Diels–Alder and the Meerwein–Ponndorf reactions [19].

## 6 Shiga University of Medical Science, Otsu

In 1975, I left the NCCRI and accepted a professorship in chemistry at the newly founded Shiga University of Medical Science. This university was founded under a then new policy of the Japanese government to increase the number of medical doctors in Japan. My main educational responsibility was to teach general chemistry to freshman and sophomores students. I was also expected to help in setting up the organization, in the design of the new building and in the procurement of instruments for this newly founded medical science university. During my first two to three years at this university, I was especially occupied with these administrative and teaching commitments and hence did not have much time to dedicate to my former research projects. However, I did make time to develop a method to evaluate the magnitude of the effect of through-space/through-bond interactions on the ionization energy. Here, all Fock matrix elements needed to be transformed from the atomic orbital (AO) basis to a localized orbital basis. By setting appropriate core resonance integrals to zero followed by diagonalization, one could obtain the change of the orbital energy in question. The method was applied in the framework of ab initio Hartree–Fock and semiempirical CNDO/2 theory to various systems with lone pairs in molecules in order to determine the relationship between the through-space/through-bond interactions and the orbital energies of lone pairs [20]. The method was also applied to the electrophilicity of the OH radical by comparing the magnitude of the electron transfer from aliphatic compounds to the OH group with that from the OH group to aliphatic compounds in hydrogen abstraction reactions using semiempirical CNDO/2 theory. As a result of these analyses, the OH radical was found to be electrophilic in nature [21]. This research was carried out mainly by Dr. H. Shinohara who later became professor of Tokyo Metropolitan University.

In 1979, the 3rd International Conference of Quantum Chemistry (ICQC) was held in Kyoto, Japan in which Prof. K. Fukui was the chairman of this conference. At this conference, I met Prof. Janos Ladik of Erlangen University in Germany. He was able to offer me a nine-month guest professor position at Erlangen University. I willingly accepted his offer and stayed from January to September of 1981 in Erlangen. While in Erlangen, I worked on the development of the use of perturbation theory to calculate the interaction energy between two nearly incommensurate polymers by using the ab initio Hartree–Fock program for periodic polymers written by Dr. Sandor Suhai who became later the professor and Head of the Department (Abteilung in German) of Molecular Biophysics and Bioinformatics at the German Cancer Research Center [Deusches Krebsforschungszentrum (DKFZ)] in Heidelberg, Germany. Dr. Suhai kindly went over the theory and details of the program with me, which made it possible for me to make further developments in this line of research [22]. He also sent one of his PhD students Gerd Räther from Heidelberg to work with me for one year in the 1990s.

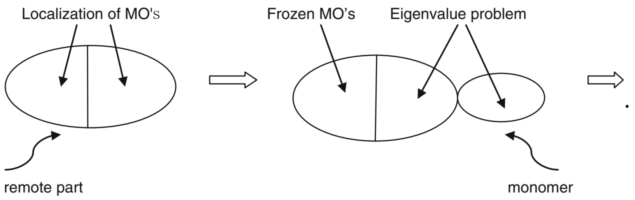
## 7 Hiroshima University

In 1982, I moved from Shiga University of Medical Science to Hiroshima University as a professor of physical chemistry in the Department of Chemistry in the Faculty of Science. I continued my previous research projects on quantitative analyses of the through-space/through-bond interaction [23] and studies of the electronic structure of various polymers [24] with some very capable and bright students. I also investigated the Peierls instability from the perspective of the phase of molecular orbitals with my PhD student Yuriko Aoki who would later became professor of materials science at Kyushu University. The energy difference between equi-bond structure and bond alternating structure in polyacetylene was explained by the phases of the HOMO and MO’s near the HOMO. The semiquantitative evaluation of this energy difference was successfully carried out by means of Hückel molecular orbital theory for a finite length of polyacetylene [25]. Moreover, we could rationalize the fact that the bond alternation is suppressed by the inter-chain interaction in terms of bonding and antibonding combinations of two molecular orbitals of the polymers concerned, that is, when antibonding combination of two HOMOs is higher than the bonding combination of two LUMOs, the bond alternation was found to be suppressed. In this way, we could understand the basis for Peierls instability in terms of concepts of molecular orbitals which are familiar to chemists, without any knowledge of solid state physics. Of course, it is best to understand both the physics and chemistry explanations, and they should of course be consistent. But in many cases, one gains additional insights by looking at alternative explanations for the same physical phenomena.

Next, we tried to evaluate theoretically the quality of explosives by means of molecular orbital methods and molecular dynamics. This research was undertaken in collaboration with Dr. Y. Kohno who was a researcher of Chugokukayaku CO., LTD in Hiroshima. We found that N–N bond lengths of HMX(Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine) polymorphs calculated by the molecular orbital methods were longer than those of crystals determined by X-ray crystallography, and that the differences in bond length between calculated and experimental ones were intimately related to impact sensitivity of the HMX polymorphs. This result suggests that N–N bonds in HMX may store a kind of strain energy and this energy may play an important role in the explosion [26].

Another important focus of my research was to establish a method to calculate the electronic structures of non-periodic polymers such as DNA and proteins. As had been stated previously, I had developed the method to calculate periodic polymers by using the tight-binding approximation in semiempirical molecular orbital methods such as CNDO/2 and had obtained satisfactory results. However, this result had not been a satisfactory one for biochemists because of the limitation that this method was confined for use on periodic systems. From the time I had this point made clear to me by my biochemist colleagues, I had been trying to establish a method for the calculation of non-periodic systems. The basic idea I had was to mimic the method of protein syntheses in living systems, that is, proteins are synthesized in living system by adding one amino acid residue at a time on the ribosome. Therefore, the idea was to first calculate the electronic structure of an oligomer using the usual molecular orbital methods, and then add the next monomer to the oligomer. We then needed to obtain the electronic structure of oligomer + monomer system (extended chain). In the first stage of this research, perturbation methods were tried with little success mainly due to problems with convergence. Divergent behavior was observed and attributed to the small magnitude of the values in the denominator originating from the nearly degenerate energy levels in the oligomers. Next, the variational method was tried. In this approach, the molecular orbitals of an oligomer are calculated followed by localization of the molecular orbitals in two parts, one of which is remote enough from the site on which a newly combined monomer could attack. Consequently, all matrix elements between molecular orbitals localized in the remote part and those of attacking monomer should be negligibly small. Thus, the molecular orbitals of the newly combined system was represented as a linear combination of localized orbitals of the oligomer and molecular orbitals of attacking monomer and an eigenvalue problem derived from the variational principle is solved after dropping the matrix elements concerned with the remote part.

This procedure is schematically described below



By repeating this procedure, we can elongate (lengthen/extend) non-periodic polymers as long as we want. Therefore, we named this method the elongation method [27–29]. It should be noteworthy that any monomers can be selected and then the electronic structure of non-periodic polymers are easily calculated. Another important characteristic of this method is that the dimension of the eigenvalue problem remains nearly constant at each elongation step, in other words, the elongation method is nothing but an order-N method. We implemented this method in various types of theoretical methods such as the extended Hückel, CNDO/2, ab initio Hartree–Fock, and DFT (density functional theory) methods and satisfactory results were obtained in each case. This research had been undertaken in collaboration with Dr. Yuriko Aoki who is now Professor of Kyushu University and her many graduate students and now even postdoctoral students and visiting professors, similar to the visiting professorship I had in Erlangen with Professor Janos Ladik and Dr. Sandor Suhai in his group. After my retirement from Hiroshima University, the elongation method has been further developed by Prof. Aoki's group at Kyushu University and more recently Prof. Gu's group at South China Normal University. The method is currently able to treat three-dimensional systems such as globular proteins. Professor Aoki is now extending the method for use in calculating linear and nonlinear frequency-dependent electric field-dependent properties and property surfaces. So, the research and development is now continuing and going strong at Kyushu University in Kasuga, Fukuoka, Japan.

## 8 Hiroshima Kokusai Gakuin University, Hiroshima

In 1998, I retired from Hiroshima University and in 1999 I moved to Hiroshima Kokusai Gakuin University in Hiroshima City to assume a professorship in the Department of Mathematics where I taught freshmen science students calculus and linear algebra after working as a part-time lecturer for one year. Hiroshima Kokusai Gakuin University is relatively small private university and my educational duties were much heavier than they were at Hiroshima University. Therefore, I didn't have as much time to devote to my research projects. In addition, I was made the Dean of the Faculty of Engineering from 2001 to 2005 and then the President of the University from 2005 to 2010. During these periods, I had to devote much of my energies to various management issues of the university. Hence, I could only carry out a limited amount of research during my 10 year period at Hiroshima Kokusai Gakuin University. When one only has very limited time to pursue one's research, one must be very selective in the choice. One of my choices during this time was to research in the molecular design of conducting polymers, that is, polyene which has two $\pi$ conjugated systems perpendicular with each other. In this polymer, I designed a system in which units of finite length of sp hybridized $\sigma$ orbitals are combined periodically with a carbon atom with $sp^2$ hybridized $\sigma$ orbitals and thus every unit has two $\pi$ conjugated systems perpendicular with each other as shown below.

$$\ldots(CH)_{2n}CH_2(CH)_{2n}CH_2(CH)_{2n}\ldots$$

In this system, the $\pi$ system has tendency to form a bond alternating structure due to the Peierls instability and another perpendicular $\pi$ system also has same tendency, but the latter $\pi$ system has a preference for the formation of double bonds different from those by the former $\pi$ system. In other words, the Peierls instabilities of two $\pi$ systems are competing with each other, and as a result of the balancing of this competition this system has no bond alternations leading to a small HOMO–LUMO gap. This inference was verified by the geometry optimization calculations with DFT calculation as well as molecular orbital calculations [30]. Consequently, I could make a proposal for the molecular design of a $\pi$ conjugated single-chain electronically conductive polymers. This was the latest of my long line of research and brought me back to full circle where one of the aims of my early research was to provide unifying principles for organic and inorganic chemistry to use in the design of their new compounds and/or experiments. By interacting with both research and industrial chemists and physicists in Japan, in Erlangen and Heidelberg in Germany and in Ithaca in New York, I came to do the things I have been trained to teach my many students to do, to apply the knowledge gained in one's fundamental research programs to solve real and practical problems in society. Any country which does so will be able to continue to develop its industrial base and also teach the fundamental and basic skills to the next generation of students and civilians to be self sustaining. The nexus between teaching, research and innovation (jobs and industry generation) has never been more important than it now is. With that I will now like to finish my scientific memoirs to date, and acknowledge those who have contributed to my scientific career and made the time go very quickly, as time flies by when one is able to do what one has a love and passion to do, as I have been blessed to be able to do for the last 50 + years.

**Acknowledgments** I greatly appreciate having had the opportunity to undertake research in the field of quantum chemistry under the stimulating guidance and mentorship of many excellent researchers, including but not limited to Prof. Kenichi Fukui, Prof. Roald Hoffmann and Prof. Janos Ladik. I am also grateful to all collaborators and undergraduate, graduate and postdoctoral students who have been involved in my research projects. I would also like to sincerely express my gratitude to my former PhD student, Prof. Yuriko Aoki at Kyushu University for her enormous endeavor to organize the publication of this special issue of this periodical, Theoretical Chemistry Accounts, with Prof. Karl James Jalkanen who undertook the editorial work (peer review process and English editing for all submissions, including this memoir manuscript, and for inviting many other international scientists (both young, middle-aged and old (retired and emeritus faculty)) who were also so kind to contribute some of their best works to this Festschrift Issue. Finally, I would like to thank Professor Chris Cramer, Editor in Chief of TCA, and Springer Verlag and their staff in Heidelberg, Steffen Pauley and Petra Treiber, for accepting the proposal of Prof. Yuriko Aoki and Prof. Karl James Jalkanen to undertake the endeavor to commemorate the occasion of my 77th birthday and recent retirement from administrative duties as President of Hiroshima Kokusai Gakuin University.

## References

1. Fukui K, Imamura A, Yonezawa T, Nagata C (1960) Bull Chem Soc Jpn 33:1591–1599
2. Mulliken RS (1952) J Amer Chem Soc 74:811–824
3. Fukui K, Imamura A, Yonezawa T, Nagata C (1961) Bull Chem Soc Jpn 34:1076–1080
4. Fukui K (1964) In: Löwdin PO, Pullman B (ed) Molecular orbitals in chemistry, physics, and biology, Academic Press, New York, pp 513–537
5. Woodward RB, Hoffmann R (1965) J Amer Chem Soc 87:395–397
6. Woodward RB, Hoffmann R (1965) J Amer Chem Soc 87:2046–2048
7. Woodward RB, Hoffmann R (1965) J Amer Chem Soc 87:2511–2513
8. Pople JA, Santry DP, Segal GA (1965) J Chem Phys 43:S129–S135
9. Pople JA, Segal GA (1965) J Chem Phys 43:S136–S151
10. Hoffmann R, Imamura A, Hehre WJ (1968) J Amer Chem Soc 90:1499–1509
11. Imamura A, Hoffmann R (1968) J Amer Chem Soc 90:5379–5385
12. Imamura A (1968) Mol Phys 15:225–238
13. Hoffmann R, Imamura A (1969) Biopolymers 7:207–213
14. Imamura A (1970) J Chem Phys 52:3168–3175
15. Fujita H, Imamura A (1970) J Chem Phys 53:4555–4566
16. McWeeny R (1956) Proc Royal Soc A 235:496–509
17. Imamura A, Fujita H (1974) J Chem Phys 61:115–125
18. Houk KN, Strozier RW (1973) J Amer Chem Soc 95:4094–4096
19. Imamura A, Hirano T (1975) J Amer Chem Soc 97:4192–4198
20. Imamura A, Ohsaku M (1981) Tetrahedron 37:2191–2195
21. Shinohara H, Imamura A, Masuda T, Kondo M (1978) Bull Chem Soc Jpn 51:1917–1922
22. Imamura A, Suhai S, Ladik J (1982) J Chem Phys 76:6067–6072
23. Kanda K, Koremoto K, Imamura A (1986) Tetrahedron 42:4169–4177
24. Aoki Y, Imamura A, Sasaki T (1988) Bull Chem Soc Jpn 61:1063–1070
25. Aoki Y, Imamura A (1995) J Chem Phys 103:663–675

26. Kohno Y, Maekawa K, Tsuchioka T, Hashizume T, Imamura A (1994) Combust Flame 96:343–350
27. Imamura A, Aoki Y, Maekawa K (1991) J Chem Phys 95:5419–5431
28. Aoki Y, Imamura A (1992) J Chem Phys 97:8432–8440
29. Aoki Y, Suhai S, Imamura A (1994) J Chem Phys 101:10808–10823
30. Imamura A, Aoki Y (2006) Int J Quantum Chem 106:1924–1933

## Appendix

Collaborators:

| | |
|---|---|
| Yuriko Aoki | 1991–2011 |
| Sandor Suhai | 1981–1999 |
| Feng Long Gu | 2000–2011 |
| Kazuyoshi Ueda | 1993–1997 |
| Hiroko Fujita | 1966–1975 |
| Yuji Kohno | 1990–1998 |

Graduate students:

| | |
|---|---|
| Hideaki Umeyama | 1967–1971 |
| Hiroyuki Shinohara | 1976–1978 |
| Terumitsu. Kakumoto | 1983–1986 |
| Yuriko Aoki | 1983–1988 |
| Masato Suzuki | 1985–1987 |
| Hiroyuki Toh | 1986–1989 |
| Kouji Maeklawa | 1989–1993 |
| Masaki Mitani | 1990–1995 |
| Youji Kurihara | 1992–1998 |
| Seiji Tani | 1984–1987 |
| Gerd Räther | (from Germany) 1998–1999 |

# Publications of Akira Imamura from 1959 to 2010

1. Fukui K, Nagata C, Yonezawa T, Imamura A (1959) Expansion Formulae of Secular Determinant in Simple LCAO MO Treatment of Aromatic Hydrocarbons. Bull Chem Soc Jpn 32:450–451
2. Fukui K, Nagata C, Yonezawa T, Imamura A (1959) Density Matrix in Simple LCAO MO Method. Bull Chem Soc Jpn 32:452–454
3. Fukui K, Imamura A, Nagata C (1960) Electronic Structure and Antifungal Activity of Quinoline and Pyridine-n-Oxide Derivatives. Bull Chem Soc Jpn 32:122–123
4. Fukui K, Nagata C, Yonezawa T, Inamoto Y, Imamura A (1960) Electronic Structure and Carcinogenic Activity of Conjugated Compounds, Substituted Aromatic Hydrocarbons, Heteroaromatic Compounds and Azo Compounds. GANN 51:67–81
5. Fukui K, Imamura A, Nagata C (1960) Relation between the Electronic Structure and Carcinogenic Activity of 4-Nitroquinoline-n-oxide and Related Compounds. GANN 51:119–123
6. Fukui K, Nagata C, Imamura A (1960) Electronic Structure and Nicotine-like Stimulant Activity in Choline Phenyl Ethers. Science 132:87–89
7. Fukui K, Imamura A, Yonezawa T, Nagata C (1960) A Quantum–Mechanical Approach to the Theory of Aromaticity. Bull Chem Soc Jpn 33:1591–1599
8. Fukui K, Nagata C, Imamura A, Tagashira Y (1961) On the Relation between Electronic Structure and Carcinogenic Activity of Urethan (Ethylcarbamate) and Related Compounds. GANN 52:127–134
9. Fukui K, Nagata C, Yonezawa T, Morokuma K, Imamura A (1961) On the Relation between the Electronic Structure and anti-Tumor Activity of Carcinostatic Compounds. GANN 52:1–14
10. Fukui K, Morokuma K, Nagata C, Imamura A (1961) Electronic Structure and Biochemical Activities in Diethyl Phenyl Phosphates. Bull Chem Soc Jpn 34:1224–1227
11. Fukui K, Imamura A, Yonezawa T, Nagata C (1961) A Theoretical Treatment of Molecular Complexes. I. Silver-Aromatic Hydrocarbon Complexes. Bull Chem Soc Jpn 34:1076–1080
12. Fukui K, Nagata C, Imamura A, Yonezawa T, Tagashira Y (1962) Relationship between the Electronic Structure and Carcinogenic Activity of Acetamidefluorene and Related Compounds. GANN 53:25–40
13. Fukui K, Imamura A, Yonezawa T, Nagata C (1962) A Theoretical Treatment of Molecular Complexes. II. Iodine-Aromatic Hydrocarbon Complexes. Bull Chem Soc Jpn. 35:33–38
14. Fukui K, Kato H, Yonezawa T, Morokuma K, Imamura A, Nagata C (1962) $\sigma$-Electronic Structure in Conjugated Systems. Bull Chem Soc Jpn 35: 38–45
15. Nagata C, Imamura A, Saito H, Fukui K (1963) Changes of $\pi$-Electron Distribution of Deoxyribonucleic Acid of the Alkylation and Their Possible Relation to the Biological Effect. GANN 54:109–117
16. Nagata C, Imamura A, Fukui K, Saito H (1963) Quantity of Charge Transfer and Carcinogenic Activity of 4-Nitroquinoline 1-Oxides and of Some Aromatic Hydrocarbons. GANN 54:401–414
17. Fukui K, Imamura A, Nagata C (1963) A Molecular Orbital Treatment of Phosphate Bonds of Biochemical Interest. II. Metal Chelates of Adenosine Triphosphate. Bull Chem Soc Jpn 36:1450–1453
18. Iguchi K, Nozaki T, Imamura A, Takahashi S (1963) The Ultraviolet Spectra of Monohalo-, Mononitro- and Monoamino-p-terphenyls. Bull Chem Soc Jpn 36:696–699
19. Naraba T, Mizushima Y, Noake H, Imamura A, Igarashi Y, Torihashi Y, Nishioka A (1965) Preparation and Electrical Properties of Polytetracyanoethylene Copper Chelate Film. Jpn J Appl Phys 4:977–986
20. Nagata C, Imamura A, Tagashira Y, Kodama M (1965) Semi-Empirical Self-Consistent Field Molecular Orbital Calculation of the Electronic Structure of the Base Components of Nucleic Acids. Bull Chem Soc Jpn 38:1638–1645
21. Nagata C, Imamura A, Tagashira Y, Kodama M, Fukuda N (1965) Quantum–Mechanical Study on the Photodimerization of Aromatic Molecules. J. theor Biol 9:357–365
22. Nagata C, Kodama M, Imamura A, Tagashira Y (1966) Interaction of Tricycloquinazoline and its Analog with DNA. GANN 57:75–84
23. Kodama M, Tagashira Y, Imamura A, Nagata C (1966) Effect of Secondary Structure of DNA upon Solubility of Aromatic Hydrocarbons. J Biochem 59:257–264

24. Imamura A, Kodama M, Tagashira Y, Nagata C (1966) The Semi-Empirical SCF Treatment of $\sigma$-$\pi$ System I. Peptide Molecule. J theor Biol 10:356–369
25. Nagata C, Kodama M, Tagashira Y, Imamura A (1966) Interaction of Polynuclear Aromatic Hydrocarbons, 4-Nitroquinoline 1-Oxides, and Various Dyes with DNA. Biopolymers 4:409–427
26. Kataoka N, Imamura A, Kawazoe Y, Chihara G, Nagata C (1966). Chem Pharm Bull 14:897–902. http://www.journalarchive.jst.go.jp/jnlpdf.php?cdjournal=cpb1958&cdvol=14&noissue=8&startpage=897&lang=en&from=jnltoc
27. Nagata C, Kataoka N, Imamura A, Kawazoe Y, Chihara G (1966) Electron Spin Resonance Study on the Free Radicals Produced from 4-Hydroxyaminoquinoline 1-Oxide and its Significance in Carcinogenesis. GANN 57:323–335
28. Nagata C, Tagashira Y, Kodama M, Imamura A (1966) Free Radical Produced by Interaction of Aromatic Hydrocarbons with Tissue Components. GANN 57:437–440
29. Sugimura T, Okabe K, Imamura A (1966) Number of Cytoplasmic Factors in Yeast Cells. Nature 212: 304–304. doi:10.1038/212304a0
30. Kataoka N, Imamura A, Kawazoe Y, Chihara G, Nagata C (1966) Electron Spin Resonance Study on the Photoinduced Radicals from Related Compounds to Carcinogenic 4-Nitroquinoline 1-Oxide. Chem Pharm Bull 14:1171–1178. http://www.journalarchive.jst.go.jp/jnlpdf.php?cdjournal=cpb1958&cdvol=14&noissue=10&startpage=1171&lang=en&from=jnltoc
31. Imamura A, Fujita H, Nagata C (1967) The Electronic Structure of Peptide and the Base Components of Nucleic Acids in the Triplet State. Bull Chem Soc Jpn 40:21–27
32. Kataoka N, Imamura A, Kawazoe Y, Chihara G, Nagata C (1967) The Structure of the Free Radical Produced from Carcinogenic 4-Hydroxyaminoquinoline 1-Oxide. Bull Chem Soc Jpn 40:62–68
33. Kataoka N, Shibata A, Imamura A, Kawazoe Y, Chihara G, Nagata C (1967) Oxidation Reaction of Carcinogenic 4-Hydroxyaminoquinoline 1-Oxide. Chem Pharm Bull 15:220–225. http://www.journalarchive.jst.go.jp/jnlpdf.php?cdjournal=cpb1958&cdvol=15&noissue=2&startpage=220&lang=en&from=jnltoc
34. Imamura A, Fujita H, Nagata C (1967) Semi-Empirical Self-Consistent Field Molecular Orbital Calculation of the Electronic Structure of the Base Pairs of Deoxyribonucleic Acid. Bull Chem Soc Jpn 40:522–526
35. Nagata C, Fujita H, Imamura A (1967) Semi-Empirical Self-Consistent Field Molecular Orbital Calculation of Transition Energy and Oscillator Strength for the Stacked Complexes of Pyrene and 3,4-Benzopyrene with DNA Bases. Bull Chem Soc Jpn 40:2564–2568
36. Hoffmann R, Imamura A, Zeiss GD (1967) The Spirarenes. J Am Chem Soc 89:5215–5220
37. Fujita H, Imamura A, Nagata C (1968) ASMO-SCF-CI Calculation on the Electronic Structures of the Bases of Nucleic Acids with Special Emphasis on the Configuration Interaction. Bull Chem Soc Jpn 41:2017–2026
38. Imamura A (1968) General Perturbation Theory for the Extended Hückel Method. Mol Phys 15:225–238. doi:10.1080/00268976800101011
39. Hoffmann R, Imamura A, Hehre WJ (1968) Benzynes, Dehydroconjugated Molecules, and the Interaction of Orbitals Separated by a Number of Intervening $\sigma$ Bonds. J Am Chem Soc 90:1499–1509
40. Imamura A, Hoffmann R (1968) The Electronic Structure and Torsional Potentials in Ground and Excited States of Biphenyl, Fulvalene, and Related Compounds. J Am Chem Soc 90:5379–5385
41. Fujita H, Imamura A, Nagata C (1969) The Electronic Structure of Base Components of Nucleic Acids and Their Tautomers Calculated by CNDO Method. Bull Chem Soc Jpn 42:1467
42. Nagata C, Ioki Y, Inomata M, Imamura A (1969) Electron Spin Resonance Study on the Free Radicals Produced from Carcinogenic Aminonaphthols and N-Hydroxy-Aminonaphthalenes. GANN 60:509–522
43. Imamura A, Fujita H, Nagata C (1969) The Electronic Structures of Glycine in the Isolated State and in Water. Bull Chem Soc Jpn 42:3118–3123
44. Hoffmann R, Imamura A (1969) Quantum Mechanical Approach to the Conformational Analysis of Macromolecules in Ground and Excited States. Biopolymers 7:207–213
45. Imamura A (1970) Electronic Structures of Polymers Using the Tight-Binding Approximation. I. Polyethylene by the Extended Hückel Method. J Chem Phys 52:3168–3175
46. Nagata C, Imamura A (1970) Electronic Structures and Mechanism of Carcinogenicity for Alkylnitrosamines. GANN 61:169–176
47. Fujita H, Imamura A, Nagata C (1970) Tautomerism of the Anticodon Base and the Code Degeneracy. J theor Biol 28:143–145
48. Fujita H, Imamura A (1970) Electonic Structures of Polymers Using the Tight-Binding Approximation. II. Polyethylene and Polyglycine by the CNDO Method. J Chem Phys 53:4555–4566
49. Odell BG, Hoffmann R, Imamura A (1970) The 2, 3-Dimethylenetetramethylene Biradical. J Chem Soc B 1675–1678

50. Imamura A, Hirano T, Nagata C, Tsuruta T (1972) Calculation of Optical Rotational Strength by Means of Various Types of Molecular Orbitals. Bull Chem Soc Jpn 45:396–401
51. Fujita H, Imamura A (1972) The Intermolecular Potential of Hydrocarbon Dimers as Examined by the Perturbation Theory Including Exchange Energy in the PPP Approximation. Bull Chem Soc Jpn 45:668–677
52. Nagata C, Nakadate M, Ioki Y, Imamura A (1972) Electron Spin Resonance Study on the Free Radical Production from N-Methyl-N'-nitro-N-nitrosoguanidine. GANN 63:471–481
53. Matsuyama A, Imamura A (1972) CNDO/2 Calculations of Hydrogen Bonding; Phenol- and p-Nitrophenol-ammonia systems. Bull Chem Soc Jpn 45:2196–2197
54. Imamura A, Fujita H, Nagata C (1972) Calculation of Chemical Shifts of Inner-Shell Electrons for the DNA Bases by the CNDO/2 Method Including the Charge Redistribution Effect. J Am Chem Soc 94:6287–6293
55. Imamura A, Fujita H, Nagata C (1972) A Molecular Orbital Study on the Alkylation and Depurination Reactions of the Base Components of Nucleic Acids. J theor Biol 36:447–457
56. Nagata C, Imamura A, Fujita H (1973) Electronic Structure of Nucleic Acid Bases: Their Spectroscopic Properties, Chemical Reactivities, and Biological Activities. Adv Biophys 4:1–69
57. Umeyama H, Imamura A, Nagata C (1973) A Molecular Orbital Study on the Enzymic Reaction Mechanism of α-Chymotrypsin. J theor Biol 41:485–502
58. Imamura A, Hirano T, Nagata C, Tsuruta T, Kuriyama K (1973) A Method of Analysis of the Rotational Strength in Terms of the Contributions from Molecular Fragments in the CNDO/2 Approximation. J Am Chem Soc 95:8621–8627
59. Imamura A, Fujita H (1974) Electronic Structures of Polymers Using the Tight-Binding Approximation. III. Density Matrix Approach to Poly-L-alanine and Polyglycine-water Complex by the CNDO/2 Method. J Chem Phys 61:115–125
60. Umeyama H, Imamura A, Nagata C (1974) Molecular Orbital Study on the Interaction between Coenzymes and Enzymes; NAD$^+$ or NADH and Dehydrogenases. J theor Biol 46:1–19
61. Fujita H, Imamura A, Nagata C (1974) A Molecular Orbital Study of Stability and the Conformation of Double-Stranded DNA-Like Polymers. J theor Biol 45:411–433
62. Imamura A, Nagata C (1974) A Molecular Orbital Study on the Chemical Reactivity and Biological Activity of N-Methyl-N'-nitro-N-nitrosoguanidine and Some Related Compounds. GANN 65:417–422
63. Umeyama H, Imamura A, Nagata C (1975) A Molecular Orbital Study on the Effects of Substituents on the Proton Transfer from Ser-195 to His-57 in the Hydrolysis of the α-Chymotrypsin. Chem Pharm Bull 23:3045–3055
64. Ioki Y, Imamura A, Nagata C, Nakadate M (1975) Photochemical Formation of Nitroxide Radicals from Carcinogenic N-Methyl-N'-nitro-N-nitrosoguanidine and Related Compounds. Photochem Photobiol 21: 387–391
65. Imamura A, Hirano T(1975) A Novel Approach to the Theory of Catalytic Activity in Terms of Molecular Orbital Mixing. J Am Chem Soc 97:4192–4198
66. Nagata C, Fujita H, Imamura A (1976) A Molecular Orbital Study on the Interaction between the Cytochrome P-450 and its Substrates. Chem Biol Interactions 12:1–12
67. Umeyama H, Imamura A, Nagata C, Nakagawa S (1977) Molecular Orbital Study of Lactate Dehydrogenase. Chem Pharm Bull 25:1685–1693
68. Yamabe T, Tanaka K, Imamura A, Kato H, Fukui K (1977) The Electronic States of $(SN)_x$ and $(SCH)_x$ Polymers. Bull Chem Soc Jpn 50:798–801
69. Shinohara H, Imamura A, Masuda T, Kondo M (1978) A Molecular Orbital Study of the Partial Reactivity of the Hydrogen of Aliphatic Compounds in the Hydrogen-Abstraction Reaction by the Hydroxyl Radical. Bull Chem Soc Jpn 51:98–102
70. Shinohara H, Imamura A, Masuda T, Kondo M (1978) A Molecular Orbital Study of the Electrophilicity of Hydroxyl Radical in Hydrogen Abstraction Reaction. Bull Chem Soc Jpn 51:1917–1922
71. Ohsaku M, Imamura A, Hirao K (1978) An Analysis of the Through-bond Interaction Using the Localized Molecular Orbitals. I. Interactions between Lone-pair Orbitals in Azines: Pyridazine, Pyrimidine, and Pyrazine. Bull Chem Soc Jpn 51:3443–3448
72. Tanaka K, Yamabe T, Fukui K, Imamura A, Kato H (1978) On the Interchain Interaction in the $(SN)_x$ Polymer. Chem Phys Lett 53:452–456
73. Umeyama H, Takeda K, Ogura H, Moriguchi I, Imamura A (1978) A Molecular Orbital Study on the n-$\pi$* Cotton Effect of ε-Caprolactam. Chem Pharm Bull 26:3440–3443. http://www.journalarchive.jst.go.jp/jnlpdf.php?cdjournal=cpb1958&cdvol=26&noissue=11&startpage=3440&lang=en&from=jnltoc
74. Ohsaku M, Imamura A (1978) Electronic Structure and Conformations of Polyoxymethylene and Polyoxyethylene. Macromol 11:970–976
75. Shinohara H, Imamura A, Masuda T, Kondo M (1979) A Molecular Orbital Study on the Partial Reactivity of Hydrogen of Various Amino Acids in

the Abstraction Reaction by Hydroxyl Radical. Bull Chem Soc Jpn 52:1–7

76. Imamura A, Hirao K (1979) A Molecular Orbital Approach to the Electrophilicity of H and OH Radicals. Bull Chem Soc Jpn 52:287–292
77. Shinohara H, Imamura A, Masuda T, Kondo M (1979) Polarity of Free Radicals in Hydrogen Abstraction Reactions. Bull Chem Soc Jpn 52:974–979
78. Ohsaku M, Imamura A, Hirao K, Kawamura T (1979) An Analysis of the Through-bond Interaction Using the Localized Molecular Orbitals. II. Long-range Proton Hyperfine Coupling in Bridgehead Alkyl Radicals: Bicyclo[1.1.1]pent-1-yl, Bicyclo[2.1.1]hex-1-yl and Bicyclo[2.2.1]hept-1-yl Radicals. Tetrahedron 35:701–706
79. Yamabe T, Tanaka K, Teramae H, Fukui K, Imamura A, Shirakawa H, Ikeda S (1979) The Electronic Structures of cis-Polyacetylene. Solid State Commun 29:329–333
80. Yamabe T, Tanaka K, Teramae H, Fukui K, Imamura A, Shirakawa H, Ikeda S (1979) Electronic Properties of Pure and Doped Polyacetylenes. J Phys C 12:L257–L262. doi:10.1088/0022-3719/12/7/003
81. Ohsaku M, Murata H, Imamura A, Hirao K (1979) A Quantitative Analysis of the Through-space and the Through-bond Interactions between Lone-pairs in Azines: Pyridazine, Pyrimidine, and Pyrazine. Tetrahedron 35:1595–1600
82. Imamura A, Koda M, Kato S (1979) A Molecular Orbital Study on the Chemical Reactivity and Biological Activity of Polycyclic Aromatic Hydrocarbon Diol-Epoxides in Connection with Bay Region Theory. GANN 70:291–296
83. Imamura A, Hirao K (1979) An Analysis of the Through-bond Interaction Using the Localized Molecular Orbitals. III. Long Range Effect of Lone Pair Orbital to the Optical Rotatory Strength of the Carbonyl n-$\pi$* Transition in 3-Ketopiperidines. Tetrahedeon 35:2243–2248
84. Imamura A, Tanaka K, Yamabe T, Fukui K (1979) Molecular Orbital Theory of the Electronic Structures of One-Dimensional Molecular Crystals. Theoret Chim Acta 54:1–14. http://www.springerlink.com/content/ql681u6581706642/fulltext.pdf
85. Shinohara H, Imamura A, Masuda T, Kondo M (1979) A Molecular Orbital Study on the Nucleophilicity and the Electrophilicity of Free Radicals in Abstraction Reactions. Bull Chem Soc Jpn 52:2801–2807
86. Shinohara H, Imamura A (1979) The Origin of the Polarity of a Radical in Hydrogen Abstraction Reaction. Bull Chem Soc Jpn 52:3265–3270
87. Akagi K, Yamabe T, Kato H, Imamura A, Fukui K (1980) Analysis of the Rotational Strength by Means of Configuration Analysis Based on the Localized Molecular Orbitals. J Am Chem Soc 102:5157–5165
88. Ohsaku M, Murata H, Imamura A, Hirao K (1980) An Analysis of the Through-bond Interaction Using the Localized Molecular Orbitals. IV. Long-range Proton Hyperfine Coupling in Exo-and Endo-Hydrogens in Bicyclo[2.1.1]hex-5-yl Radical. Tetrahedron 36:177–182
89. Imamura A, Koda M, Kato S (1980) A Molecular Orbital Study on the Carcinogenicity of Various Polycyclic Aromatic Hydrocarbon Diol-Epoxides. GANN 71:737–738
90. Ohsaku M, Imamura A (1980) CNDO/2 Calculations of the Relative Stability of Poly(L-proline I) and Poly(L-proline II). Int J Biol Macromol 2:347–354
91. Ohsaku M, Murata H, Imamura (1980) Long-range Resonance and Electrostatic Interactions in Poly-L-proline by the CNDO/2 Procedure. Int J Biol Macromol 2:381–382
92. Imamura A, Ohsaku M (1981) An Analysis of the Through-bond Interaction Using the Localized Molecular Orbitals with Ab Initio Calculations. I. Lone-Pair Orbital Interactions in cis- and trans-Hydrazines. Tetrahedron 37:2191–2195
93. Ohsaku M, Izuoka T, Imamura A, Murata H (1981) Conformational Stability of Poly(trimethylene oxide) by CNDO/2 Calculations. Polymer 22:624–626
94. Ohsaku M, Murata H, Imamura A (1981) Electronic and Molecular Structures of $(HCN)_n$ Polymers. Eur Polymer J 17:327–332
95. Ohsaku M, Sasaki T, Murata H, Imamura A (1981) Electronic and Molecular Structures of $(HCN)_n$ Polymers: $[(HCN)_3]_n$. Eur Polymer J 17:913–917
96. Ohsaku M, Shigemi S, Murata H, Imamura A (1981) A Quantitative Analysis of the Through-space and the Through-bond Interactions between Lone-Pairs and $\sigma$-Frames: s-Triazine and s-Tetrazine. Tetrahedron 37:297–306
97. Imamura A, Tachibana A, Ohsaku M (1981) An Analysis of the Through-bond Interaction Using the Localized Molecular Orbitals with ab Initio Calculations. II. Lone-pair Orbital Energies in Bicyclo Compounds: 7-Azabicyclo[2.2.1]heptane and 2-Azabicyclo[2.2.2]octane, and their N-Methyl Derivatives. Tetrahedron 37:2793–2796
98. Ohsaku M, Hatamoto T, Imamura A, Murata H (1981) Electronic and Molecular Structures of Poly(hydroxymethylene) and Poly(vinyl alcohol). Polymer J 13:733–740
99. Ohsaku M, Murata H, Imamura A, Tachibana A (1981) Molecular and Electronic Structures of Polythiomethylene(PTM). Polymer 22:1346–1348

100. Imamura A, Suhai S, Ladik J (1982) Perturbational Approach to the Interaction between Two Nearly Incommensurable Polymers. J Chem Phys 76:6067–6072
101. Ohsaku M, Kawamura T, Murata H, Imamura A (1982) CNDO/2 Calculations of the Relative Stability of Poly($\gamma$-hydroxy-L-proline). Int J Biol Macromol 4:37–42
102. Ohsaku M, Murata H, Imamura A (1982) CNDO/2 Calculations of the Relative Stability of the Goniomers in Poly(DL-alanine). Int J Biol Macromol 4:103–106
103. Ohsaku M, Hatamoto T, Murata H, Imamura A (1982) Stability of the Crystal Structures of Poly(-vinyl alcohol) (PVA) by CNDO/2 Calculations. Polymer 23:776–778
104. Imamura A, Kurumi Y, Danzuka T, Kodama M, Kawachi T, Nagao M (1983) Classification of Compounds by Cluster Analysis of Ames Test Data. GANN 74:196–204
105. Imamura A, Ohsaku M (1983) A Molecular Orbital Treatment on the Reactivity of Some Polycyclic Aromatic Hydrocarbon Diol-Epoxides. J theor Biol 102:511–519
106. Imamura A, Ohsaku M (1983) Theoretical Study on the Nature of the Hydrogen Bonds in an $\alpha$-helical Polymer and its Model Systems. Polymer 24:1639–1643
107. Imamura A, Ohsaku M, Akagi K (1983) An Analysis of the Through-bond Interaction Using the Localized Molecular Orbitals with ab Initio Calculations. III. Lone-pair Orbital Interaction in 1,4-Diazabicyclo[2.2.2]octane and its Model Molecules. Tetrahedron 39:1291–1297
108. Teramae H, Yamabe T, Satoko C, Imamura A (1983) Energy Gradient in the ab initio Hartree–Fock Crystal-Orbital Formalism of One-Dimensional Infinite Polymers. Chem Phys Lett 101:149–152
109. Ohsaku M, Imamura A (1983) Relative Stability of Poly($\beta$-hydroxy-L-proline). Int J Biol Macromol 5:322–324
110. Teramae H, Yamabe T, Imamura A (1983) Ab Initio Effective Core Potential Studies on Polymers. Theor Chem Acc 64:1–12
111. Saito K, Kakumoto T, Kuroda H, Torii S, Imamura A (1984) Thermal Unimolecular Decomposition of Formic Acid. J Chem Phys 80:4989–4996
112. Ohsaku M, Imamura A (1984) Conformational Stability of Poly(trimethylene sulphide). Polymer 25:511–512
113. Teramae H, Yamabe T, Imamura A (1984) Ab Initio Studies on the Geometrical and Vibrational Structures of Polymers. J Chem Phys 81:3564–3572
114. Ohsaku M, Ichiishi T, Imamura A, Hayashi M (1984) Ab Initio Self-Consistent Field MO Calculations of Ethanethiol and Ethanol. Bull Chem Soc Jpn 57:2791–2796
115. Ohsaku M, Imamura A (1984) Conformational Analyses of Poly(methylene disulphide). Polymer Commun 25:251–253
116. Ohsaku M, Izumi J, Imamura A (1984) Electronic Structures of Collagen Model Polymers: $(\text{Gly-Pro})_n$, $(\text{Gly-Hyp})_n$, $(\text{Ala-Pro})_n$, $(\text{Ala-Hyp})_n$, $(\text{Gly-Pro-Gly})_n$, $(\text{Gly-Hyp-Gly})_n$, $(\text{Gly-Pro-Pro})_n$, $(\text{Gly-Pro-Hyp})_n$. Int J Biol Macromol 6:234–240
117. Ohsaku M, Taketoshi M, Imamura A (1985) A Theoretical Study on the Inter-chain Interactions in Poly(amino acid)s. J Mol Struct (Theochem) 119:307–317
118. Ohsaku M, Imamura A (1985) Ab Initio SCF MO Conformational Analysis of 2,3-Butadien-1-ol. J Mol Struct (Theochem) 119:319–327
119. Kakumoto T, Saito K, Imamura A (1985) Thermal Decomposition of Formamide: Shock Tube Experiments and ab Initio Calculations. J Phys Chem 89:2286–2291
120. Saito K, Kakumoto T, Nakanishi Y, Imamura A (1985) Thermal Decomposition of Formaldehyde at High Temperatures. J Phys Chem 89:3109–3113
121. Imamura A, Aoki Y (1985) A Novel Iterative Transfer Perturbation Method and Its Application to the Extended Hückel Method. Bull Chem Soc Jpn 58:1376–1379
122. Imamura A, Aoki Y, Suhai S, Ladik J (1985) Perturbational Approach to the Interaction between a Polymer and a Small Molecule. J Chem Phys 83:5727–5734
123. Aoki Y, Imamura A, Teramae H (1985) A Trough Space/Bond Interaction Analysis on the Shape of Band Structure of Polynitrilomethylidyne. Bull Chem Soc Jpn 58:2737–2745
124. Imamura A, Tani S, Taketoshi M, Danzuka T (1985) The Relation between Ames Test Data and Electronic Structure for a Series of Benzidine Derivatives Investigated by Using Cluster Analysis. GANN 76:937–945
125. Ohsaku M, Imamura A (1985) An ab initio SCF MO Study of Conformational Stability in Ethyl Methyl Sulphide. Mol Phys 55:331–339
126. Imamura A, Okajima T, Kanda K (1986) A Molecular Orbital Approach to the Effect of Acid and Base

on Mutarotation of D-Glucose. Bull Chem Soc Jpn 59:943–945

127. Kanda K, Imamura A (1986) Theoretical Study on the Stability of Hexafluoro Dewar Benzene. J Mol Struct (Theochem) 136:111–119
128. Saito K, Ito R, Kakumoto T, Imamura A (1986) The Initial Process of the Oxidation of the Methyl Radical in Reflected Shock Waves. J Phys Chem 90:1422–1427
129. Aoyama T, Imamura A, Matsubara H, Imamura T, Sugahara T (1986) Computer Simulation of Radiation-Induced Late Effects by "System Dynamics". J Radiat Res 27:230–239
130. Saito K, Ueda Y, Ito R, Kakumoto T, Imamura A (1986) Measurements of the Bimolecular Rate Constants for $S + O_2 \rightarrow SO + O$ and $CS_2 + O_2 \rightarrow CS + SO_2$ at High Temperatures. Int J Chem Kinet 18:871–884
131. Kanda K, Koremoto T, Imamura A (1986) An Analysis of the Through-bond Interaction Using the Localized Molecular Orbitals with ab Initio Calculations. IV. Role of Relay Orbitals in Perpendicular $\pi$-Systems. Tetrahedron 42:4169–4177
132. Imamura A, Aoki Y (1986) An Iterative Transfer Perturbation Method and its Application to the Interaction between a Polymer and a Small Molecule. Chem Phys Lett 130:390–394
133. Kakumoto T, Ushirogouchi T, Saito K, Imamura A (1987) Isomerization of Allene $\rightleftarrows$ Propyne in Shock Waves and ab initio Calculations. J Phys Chem 91:183–189
134. Kakumoto T, Saito K, Imamura A (1987) Unimolecular Decomposition of Oxalic Acid. J Phys Chem 91:2366–2371
135. Imamura A, Aoki Y (1987) Iterative Transfer Perturbation Method and its Applications to the Interaction between a Polymer and Small Molecules. Synthetic Metals 17:135–141
136. Toh H, Imamura A, Kanda K (1987) Role of $Mg^{2+}$ in the Ribozyme System. FEBS Lett 219:279–282
137. Imamura A, Aoki Y (1987) Perturbational Approach to Aperiodicity of Polymer Systems. Int J Quantum Chem 32 (Quantum Chemistry Symposium) 21:137–151. doi:10.1002/qua.560320717
138. Tani S, Imamura A, Kanda (1987) A Molecular Orbital Study of the Metabolic Pathway with Hydroquinone Intermediate from Benzene as Carcinogen. J Biol Phys 15:17–21
139. Aoki Y, Imamura A, Sasaki T (1988) A Through Space/Bond Interaction Analysis of the Shape of the Band Structure of Polyacetylene. Bull Chem Soc Jpn 61:1063–1070
140. Aoki Y, Imamura A, Morokuma K (1988) Self-Consistent-Field Iterative Transfer Perturbation Method and its Application to the Interaction between a Polymer and a Small Molecule. J Chem Phys 89:1147–1152
141. Saito K, Makishita K, Kakumoto T, Sasaki T, Imamura A (1988) Unimolecular Thermal Reaction of Formaldoxime at High Temperatures: Experiments and Calculations. J Phys Chem 92:4371–4374
142. Imamura A, Tani S, Kanda K (1988) Molecular Orbital Study on the Metabolic Pathway through the Diol Epoxide Form of Carcinogenic Benzene in Comparison with Benzo[a]pyrene. J theor Biol 135:215–218
143. Toh H, Imamura A, Kanda K (1989) Whether $Zn^{2+}$ for the Polymerase System was Selected Inevitably or by Historical Accident. J theor Biol 136: 79–85
144. Aoki Y, Imamura A, Morokuma K (1989) Self-Consistent-Field Variational Approach to the Interaction between a Polymer and a Small Molecule. Theor Chem Acc 75:247–260
145. Imamura A, Ye K, Taketoshi M (1989) A Theoretical Study of the Ionized State of Polymers with the Localized Molecular Orbital Method. Bull Chem Soc Jpn 62:979–984
146. Suzuki M, Imamura A (1989) Application of the Recursion Method to the Study of the End Effects on the Bond Length Alternation in Polyacetylene. Int J Quantum Chem 35: 613–628
147. Aoki Y, Watanabe E, Imamura A (1989) An Energy-Decomposition Technique for the Analysis of Band Structure and its Application to Polyphosphazene and its Halogenated Derivatives. J Mol Struct (Theochem) 188:321–335
148. Tani S, Imamura A, Kanda K (1989) Kinetic Approach with ab initio MO Method on Ionic Selectivity and Size in Sodium Channel. J theor Biol 140:519–536
149. Ushio T, Kato T, Ye K, Imamura A (1989) An Analysis of the Through-bond Interaction Using the Localized Molecular Orbitals with ab initio Calculations. V. HOMO Energy Levels of Many Propellane Compounds. Tetrahedron 45:7743–7758
150. Saito K, Adachi K, Watanabe W, Shimofuji K, Imamura A (1990) The Thermal Unimolecular Decomposition of 3,4-Dihydro-2H-pyran behind Reflected Shock Waves. Chem Phys Lett 165:383–385
151. Saito K, Mochizuki Y, Yoshinobu I, Imamura A (1990) On the Thermal Unimolecular Decomposition of Propynal. Chem Phys Lett 167:347–350
152. Seki K, Tanaka H, Ohta T, Aoki Y, Imamura A, Fujimoto H, Yamamoto H, Inokuchi H (1990)

Electronic Structure of Poly(tetrafluoroethylene) Studied by UPS, VUV Absorption, and Band Calculations. Physica Scripta 41:167–171

153. Hayashi S, Aoki Y, Imamura A (1990) A Study Using a Through-Space/Bond Interaction Analysis for the Band Structures of Substituted Polyacetylene-Be Systems. Synthetic Metals 36:1–25
154. Watanabe E, Imamura A (1990) A Study on Peierls Instability in Quasi-One-Dimensional-System with Interchain-Interactions. Semi-Empirical Self-Consistent-Field Molecular Orbital Approach. Bull Chem Soc Jpn 63:1678–1683
155. Aoki Y, Imamura A, Murata I (1990) A Molecular Orbital Study on the Electron Donating and Accepting Abilities of non-Alternant Polycyclic Conjugated Hydrocarbons. Tetrahedron 46:6659–6672
156. Saito K, Sasaki T, Yoshinobu I, Imamura A (1990) Thermal Decomposition of Ethyl Acetate. Branching ratio of the Competing Paths in the Pyrolysis of the Produced Acetic Acid. Chem Phys Lett 170: 385–388
157. Akagi K, Kadokura T, Shirakawa H, Teramae H, Imamura A (1990) Geometrical and Electronic Structures of Polyacetylene Chlorinated via Prolonged Chemical Doping. Int J Quantum Chem 24:41–50
158. Koshi M, Yoshimura M, Fukuda K, Matsui H, Saito K, Watanabe M, Imamura A, Chen C (1990) Reactions of N($^4$S) atoms with NO and $H_2$. J Chem Phys 93:8703–8708
159. Hayashi S, Yabushita S, Imamura A (1991) Ab initio Calculations of Linear and Nonlinear Polarizabilities in the Side-Chain Direction on the Conjugated Polymers. Chem Phys Lett 179:405–409
160. Shimofuji K, Saito K, Imamura A (1991) Unimolecular Thermal Decomposition of Ethyl Vinyl Ether and the Consecutive Thermal Reaction of the Intermediary Product Acetaldehyde: Shock Wave Experiment and ab Initio Calculation. J Phys Chem 95:155–165
161. Aoki Y, Imamura A (1991) Self-Consistent-Field Perturbational Approach to Aperiodic Polymers. J Mol Struct (Theochem) 235:95–105
162. Imamura A, Aoki Y, Maekawa K (1991) A Theoretical Synthesis of Polymers by Using Uniform Localization of Molecular Orbitals: Proposal of an Elongation Method. J Chem Phys 95:5419–5431
163. Sugihara Y, Yagi T, Murata I, Imamura A (1992) 1-Phenylthieno[3,4-d]borepine: A New 10 $\pi$ Electron System Isoelectronic with Azulene. J Am Chem Soc 114:1479–1481
164. Hayashi S, Imamura A (1992) A Study of the Polarization Reversal in Poly(vinylidene Fluoride) Using Molecular Orbital Calculations. J Polym Sci B 30:769–773
165. Kohno Y, Maekawa K, Azuma N, Tsuchioka T, Hashizume T, Imamura A (1992) Ab Initio calculations for a relationship between impact sensitivity and molecular structure in HMX polymorphs. Kogyo Kayaku 53:227–237
166. Aoki Y, Imamura A (1992) A Simple Treatment to Design NBMO Degenerate Systems in Alternant and non-Alternant Hydrocarbons. Theor Chem Acc 84:155–180
167. Aoki Y, Imamura A (1992) Local Density of State of Aperiodic Polymers Using the Localized Orbitals from an ab initio Elongation Method. J Chem Phys 97:8432–8440
168. Maekawa K, Imamura A (1993) Stationary Conditions of the Electronic Structures Against the Extension of Molecular Systems and their Application to the Elongation Method. J Chem Phys 98:534–542
169. Ueda K, Ochiai H, Imamura A, Yamaoka K (1993) An Observation of the Electric Birefringence Signal of $\kappa$-Carrageenan Gel. Chem Lett 601–604
170. Maekawa K, Imamura A (1993) Stationary Space Analysis of the Electronic Structure of a Polymer System: From Cluster Model to Cluster-Series Model. J Chem Phys 98:7086–7091
171. Itaya T, Ueda K, Ochiai H, Imamura A (1993) Binding of Hydrophobic Counterions by Polyelectrolyte and Their Hydrophobic Association around Polyion. Polymer J 25:545–552
172. Suenobu K, Tani S, Imamura A (1993) An ab initio Molecular Orbital Study on Effect of Electric Field Strength on Ionic Selectivity of the Sodium Channel. J theor Biol 161:395–403
173. Imamura A, Mitani M (1993) A study of the Crystal Growth Process by Using the Elongation Method. New Func Mater C 83–88
174. Maekawa K, Imamura A (1993) Electronic Structures around the Local Defects in all-trans-Polyacetylene: An Analysis by the Cluster-Series Model. Int J Quantum Chem 47:449–467
175. Kohno Y, Maekawa K, Tsuchioka T, Hashizume T, Imamura A (1993) A Molecular Orbital Study on the Effects of Electron Correlation on the Unique N–N Bond in Nitramines. Chem Phys Lett 214:603–608
176. Itaya T, Ochiai H, Ueda K, Imamura A (1993) Stacking Interaction of Naphthalenesulfonate Ions around Poly (allylammonium) Cation. Macromolecules 26:6021–6026
177. Kubota H, Aoki Y, Imamura A (1994) Ab initio Study of the Relationship between the Pressure and

the Change in the Dipole Moment of a Molecule in a Ferroelectric Crystal. Bull Chem Soc Jpn 67:13–20

178. Itaya T, Ochiai H, Aoyama T, Ueda K, Imamura A (1994) Association of Hydrophobic Counterions in Aqueous Solution of Poly(allylammonium) Chloride: Comparison between p-n-Propylbenzenesulfonate and p-iso-Propylbenzenesulfonate Ions. J Polym Sci B 32:171–177
179. Mitani M, Aoki Y, Imamura A (1994) A Novel Molecular Orbital Method for the Calculations of Polymer Systems with Local Aperiodic Part: The Combination of the Elongation Method with the Supercell Method. J Chem Phys 100:2346–2358
180. Ueda K, Sato S, Ochiai H, Imamura A, Yamaoka K (1994) An Investigation of the Ionic Polarization of Carrageenans with Different Charge Densities. Chem Lett 763–766
181. Kohno Y, Maekawa K, Tsuchioka T, Hashizume T, Imamura A (1994) A Relationship between the Impact Sensitivity and the Electronic Structures for the Unique N–N Bond in the HMX Polymorphs. Combust Flame 96:343–350
182. Itaya T, Ochiai H, Ueda K, Imamura A (1994) Aggregation of Polycation and Surfactant Anion Studied by Energy Transfer from 2-Naphthalenesulfonate Ion to 1-Pyrenesulfonate Ion. Polymer 35:2004–2006
183. Itaya T, Kawabata Y, Ochiai H, Ueda K, Imamura A (1994) Charge-Transfer Complexation in Aqueous Polyelectrolyte Solution. I. Complexation between Dimethoxyanthracenesulfonate Ion and Anthraquinonesulfonate Ion. Bull Chem Soc Jpn 67:1538–1543
184. Ueda K, Ochiai H, Imamura A, Nakagawa S (1994) Molecular Mechanics and Molecular Dynamics Simulation on the Conformation of Dimer Units of Carrageenan in Water. Kobunshi Ronbunshu 51:400–408
185. Itaya T, Kawabata Y, Ochiai H, Ueda K, Imamura A (1994) Charge-Transfer Complexation in Aqueous Polyelectrolyte Solution. II. Interaction between Polycations and CT Complexes. Bull Chem Soc Jpn 67:2047–2052
186. Imamura A, Aoki Y, Nishimoto K, Kurihara Y, Nagao A (1994) Calculations of the Electronic Structure of Various Aperiodic Polymers by an Elongation Method. Int J Quantum Chem 52:309–319
187. Y. Sugihara, R. Miyatake, T. Yagi, I. Murata, M. Jinguji, T. Nakazawa and A. Imamura, Thienoborepins: Conjugation Characteristics in Boron Heterocycles. Tetrahedron 50, 6495–6504 (1994).
188. Mitani M, Imamura A (1994) Application of the Elongation Method to the Calculation of Electronic Structures of the Interface and the Local Defect states in a Polymer: An Analysis of the Periodicity in the Electronic States of a Nonperiodic Polymer by Using the Cluster-Series Calculation. J Chem Phys 101:7712–7728
189. Aoki Y, Suhai S, Imamura A (1994) An Efficient Cluster Elongation Method in Density Functional Theory and its Application to Poly-Hydrogen-Bonding Molecules. J Chem Phys 101:10808–10823
190. Aoki Y, Suhai S, Imamura A (1994) A Density Functional Elongation Method for the Theoretical Synthesis of Aperiodic Polymers. Int J Quantum Chem 52:267–280
191. Ueda K, Ochiai H, Imamura A, Nakagawa S (1995) An Investigation of the Conformation of $\beta$-Carrageenan by Molecular Mechanics and Molecular Dynamics Simulations. Bull Chem Soc Jpn 68:95–106
192. Mitani M, Aoki Y, Imamura A (1995) Electronic Structures of Large, Extended, Nonperiodic Systems by Using the Elongation Method: Model Calculations for the Cluster Series of a Polymer and the Molecular Stacking on a Surface. Int J Quantum Chem 54:167–196
193. Sugihara Y, Miyatake R, Murata I, Imamura A (1995) 5-Methyl-1-phenylpyrrolo[3,4-d]borepin: A Polarized Aromatic Molecule. J Chem Soc Chem Commun 1249–1250
194. Mitani M, Imamura A (1995) A General Quantum Chemical Approach to Study the Locally Perturbed Periodic Systems: A New Development of the ab initio Crystal Elongation Method. J Chem Phys 103:663–675
195. Aoki Y, Imamura A (1995) An Analytical Hückel-Type Approach to the Relationship between Peierls Instability in Polyenes and Interchain Interaction. J Chem Phys 103:9726–9737
196. Kawabata Y, Itaya T, Sasaki Y, Ochiai H, Ueda K, Imamura A (1995) Effects of Polyelectrolytes on the Complexation between Pyrenesulfonate and Anthraquinonesulfonate Ions. Polymer J 27:542–546
197. Imamura A, Kubota H, Ogawa Y, Aoki Y (1996) Molecular Orbital Study of the Ferroelectricity of Odd Nylons. Mol Cryst Liq Cryst 278:99–109
198. Kohno Y, Ueda K, Imamura A (1996) Molecular Dynamics Simulations of Initial Decomposition Process on the Unique N–N Bond in Nitramines in the Crystalline State. J Phys Chem 100:4701–4712
199. Kawabata Y, Itaya T, Sasaki Y, Ochiai H, Ueda K, Imamura A (1996) Charge-Transfer Complexation in Aqueous Polyelectrolyte Solution. III. Complexation between Pyrenesulfonate or Anthracenesulfonate

and Anthraquinonesulfonate Ions. Bull Chem Soc Jpn 69:2453–2459

200. Aoki Y, Tada T, Imamura A (1997) Molecular Orbital Approach to the Peierls Instability in Polyenes and its Application to Model Crystals of Charge-Transfer Complexes. Int J Quantum Chem 64:325–336
201. Mitani M, Aoki Y, Imamura A (1997) Geometry Optimization of Polymers by the Elongation Method. Int J Quantum Chem 64:301–323
202. Kawabata Y, Itaya T, Sasaki Y, Ochiai H, Ueda K, Imamura A (1997) Effects of Acceptor Structure on Charge-Transfer Complexation in Aqueous Polyelectrolyte Solution. Polymer J 29:211–217
203. Imamura A, Ohtani H, Aoki Y (1997) Imamura A, Ohtani H, Aoki Y (1997) Model Calculations of the Intrinsic Reaction Coordinate for the Ion Permeation of Sodium Channels. In Sokabe M, Auerbach A, Sigworth F (ed) Progress in Cell Research: Towards Molecular Biophysics of Ion Channels, Elsevier, Amsterdam, 6:253–259
204. Kurihara Y, Aoki Y, Imamura A (1997) Calculations of the Excitation Energies of all-trans and 11,12s-dicis Retinals Using Localized Molecular Orbitals Obtained by the Elongation Method. J Chem Phys 107:3569–3575
205. Imamura A, Aoki Y (1997) An Elongation Method to Calculate the Electronic Structure of non-Periodical and Periodical Polymers. Advances in Colloid and Interface Science 71–72:147–164. doi: 10.1016/S0001-8686(97)90015-4
206. Ueda K, Sato S, Ochiai H, Imamura A (1997) Ionic Polarization of Carrageenans with Different Charge Densities as Studied by Electric Birefringence Measurements. J Phys Chem B 101:3653–3664
207. Kurihara Y, Aoki Y, Imamura A (1998) Calculations of Phase Transition of Polydiacetylenes Using Localized Molecular Orbitals by Elongation Method. J Chem Phys 108:10303–10308
208. Tada T, Aoki Y, Imamura A (1998) The Contributions of Chalcogen to the Peierls Instability in Model Crystals of Charge-Transfer Complexes. Synthetic Metals 95:169–177
209. Yamazaki T, Aoki Y, Imamura A (1998) A Method for Calculating Electric Dipole Transition Moments Using Small CI Spaces Based on the Concept of Interaction Frontier Orbitals. Chem Phys Lett 295:431–438
210. Ueda K, Imamura A, Brady JW (1998) Molecular Dynamics Simulation of a Double-Helical $\beta$-Carrageenan Hexamer Fragment in Water. J Phys Chem A 102:2749–2758
211. Ueda K, Itoh M, Matsuzaki Y, Ochiai H, Imamura A (1998) Observation of the Molecular Weight Change during the Helix-Coil Transition of $\kappa$-Carrageenan Measured by the SEC-LALLS Method. Macromolecules 31:675–680
212. Imamura A, Orimoto Y, Aoki Y (1999) Molecular and Electronic Structures of Bipolaron in Poly-para-phenylene in Terms of Molecular Orbitals Symmetry.Theor Chem Acc 102:180–187
213. Räther G, Aoki Y, Imamura A (1999) Performance of the Elongation Method with Larger Basis Sets. Int J Quantum Chem 74:35–47
214. Aoki Y, Imamura A (1999) A Simple Rule to Find Non-Disjoint NBMO Degenerate Systems for Designing High-Spin Organic Molecules. Int J Quantum Chem 74:491–502
215. Imamura A, Sugiyama H, Orimoto Y, Aoki Y (1999) Ab Initio Through Space/Bond Interaction Analysis on the Stereoelectronic Effect by Modifying the Exponents of the Basis Set. Int J Quantum Chem 74:761–768
216. Ladik J, Imamura A, Aoki Y, Ruiz MBRY, Otto P (1999) Approximate Methods of the Calculation of Effective Energies in Disordered Chains I. Comparative Theoretical Study of the Energy Properties of Structural Isomers of Polypropene. J Mol Struct (Theochem) 491:49–55
217. Tamura H, Zhou H, Sugisato K, Yokoi Y, Takami S, Kubo M, Teraishi K, Miyamoto A, Imamura A, Gamo MN, Ando T (2000) Periodic density-functional study on oxidation of diamond (100) surfaces. Phys Rev B 61:11025–11033
218. Kim M, Lee M, Kim U, Kimura M, Aoki Y, Imamura A (2001) Theoretical Synthesis of Poly-(2-hydroxyethylenemethacrylate) by Uniform Localization of Molecular Orbitals Calculation. J Polym Sci A 39:2677–2682
219. Wan X, Yoshizawa K, Ohashi N, Endou A, Takami S, Kubo M, Miyamoto A, Imamura A (2001) A Theoretical Study of Interaction of Oxygen with Noble Metal Clusters. Scripta Mater 44:1919–1923
220. Inaba Y, Onozu T, Takami S, Kubo M, Miyamoto A, Imamura A (2001) Computational Chemistry Study on Crystal Growth of InGaN/GaN. Jpn J Appl Phys 40:2991–2995
221. Fushimi M, Ando M, Kurokawa H, Zhou H, Takami S, Kubo M, Imamura A, Miyamoto A (2002) Molecular Dynamics Study of Propylene Polymerization on Ziegler–Natta Catalyst. Kobunshi Ronbunshu 59:224–229
222. Sugiki S, Aoki Y, Imamura A (2002) A quantum chemical study on the phase transition from a $\pi$-conjugated stacking system to a covalent bonding system. J Mol Struct (Theochem) 579:45–52

223. Yokosuka T, Kurokawa H, Takami S, Kubo M, Miyamoto A, Imamura A (2002) Development of New Tight-binding Molecular Dynamics Program to Simulate Chemical–Mechanical Polishing Processes. Jpn J Appl Phys 41:2410–2413
224. Elanany M, Selvam P, Yokosuka T, Takami S, Kubo M, Imamura A, Miyamoto A (2003) A Quantum Molecular Dynamics Simulation Study of the Initial Hydrolysis Step in Sol–Gel Process. J Phys Chem B 107:1518–1524
225. Suzuki K, Kuroiwa Y, Takami S, Kubo M, Miyamoto A, Imamura A (2003) Tight-binding quantum chemical molecular dynamics study of cathode materials for lithium secondary battery. Solid State Ionics 152–153:273–277
226. Sakata K, Yokosuka T, Kurokawa H, Takami S, Kubo M, Imamura A, Shinmura T, Kanoh M, Miyamoto A (2003) Quantum Chemical Molecular Dynamics Simulation of the Plasma Etching Processes. Jpn J Appl Phys 42:1859–1864
227. Yokosuka T, Sakata K, Kurokawa H, Takami S, Kubo M, Imamura A, Kitahara Y, Kanoh M, Miyamoto A (2003) A Theoretical Study on the Realistic Low Concentration Doping in Silicon Semiconductors by Accelerated Quantum Chemical Molecular Dynamics Method. Jpn J Appl Phys 42:1877–1881
228. Yokosuka T, Sakata K, Kurokawa H, Takami S, Kubo M, Imamura A, Miyamoto A (2003), Quantum Chemical Molecular Dynamics Studies on the Chemical Mechanical Polishing Process of Cu Surface. Jpn J Appl Phys 42:1897–1902
229. Luo Y, Selvam P, Ito Y, Takami S, Kubo M, Imamura A, Miyamoto A (2003), Ring Opening of Methylenecyclopropane over Lanthanocene Catalyst: A Quantum-Chemical Molecular Dynamics Simulation Study. Organometallics 22:2182–2183
230. Mukawa T, Goto T, Nariai H, Aoki Y, Imamura A, Takeuchi T (2003) Novel strategy for molecular imprinting of phenolic compounds utilizing disulfide templates. J Pharm Biomed Anal 30:1943–1947
231. Kawabata Y, Itaya T, Ueda K, Ochiai H, Aoki Y, Imamura A (2003) Novel-Type Charge-Transfer Complex Formation between Indoxyl Sulfate and Anthraquinonesulfonate Ions in an Aqueous Polyelectrolyte Solution. Polym J 35:50–55
232. Gu FL, Aoki Y, Imamura A, Bishop DM, Kirtman B (2003) Application of the elongation method to nonlinear optical properties: finite field approach for calculating static electric (hyper) polarizabilities. Mol Phys 101:1487–1494
233. Kawabata Y, Itaya T, Ueda K, Aoki Y, Imamura A (2003) A Theoretical Treatment of Charge-Transfer Interaction in an Aqueous Solution of Polyelectrolyte. Polym J 35:573–577
234. Kubo M, Ando M, Sakahara S, Jung C, Seki K, Kusagaya T, Endou A, Takami S, Imamura A, Miyamoto A (2004) Development of tight-binding, chemical-reaction-dynamics simulator for combinatorial chemistry. Appl Surface Sci 233:188–195
235. Tada T, Aoki Y, Imamura A (2004) An analytical molecular orbital approach in Tetrathiafulvalene Tetracyanoquinodi-methane (TTF-TCNQ). Mol Phys 102:1891–1901
236. Gu FL, Aoki Y, Korchowiec J, Imamura A, Kirtman B (2004) A new localization scheme for the elongation method. J Chem Phys 121:10385–10391
237. Ohnishi S, Gu FL, Naka K, Imamura A, Kirtman B, Aoki Y (2004) Calculation of Static (Hyper)Polarizabilities for $\pi$-Conjugated Donor/Acceptor Molecules and Block Co-Polymers by the Elongation Finite-Field Method. J Phys Chem A 108:8478–8484
238. Korchowiec J, Gu FL, Imamura A, Kirtman B, Aoki Y (2005) Elongation Method with Cut-off Technique for Linear SCF Scaling. Int J Quantum Chem 102:785–794
239. Suzuki A, Selvam P, Kusagaya T, Takami S, Kubo M, Imamura A, Miyamoto A (2005) Chemical Reaction Dynamics of PeCB and TCDD Decomposition: A Tight-Binding Quantum Chemical Molecular Dynamics Study with First-Principles Parametrization. Int J Quantum Chem 102:318–327
240. Imamura A, Aoki Y (2006) Molecular design of $\pi$-conjugated single-chain electronically conductive polymer. Int J Quantum Chem 106:1924–1933
241. Orimoto Y, Gu FL, Imamura A, Aoki Y (2007) Efficient and accurate calculations on the electronic structure of B-type poly(dG)-poly(dC) DNA by elongation method: First step toward the understanding of the biological properties of aperiodic DNA. J Chem Phys 125:215104
242. Aoki Y, Gu FL, Orimoto Y, Suhai S, Imamura A (2007) Elongation Method Applied to Aperiodic Systems—Random Polypeptides, High Spin Alignment, Polymer in Solvent, and DNA. In: Maroulis G, Simos TE (ed) AIP Conference Proceedings 963: Computational Methods in Science and Engineering: Theory and Computation: Old Problems and New Challenge, Lectures Presented at the ICCMSE 2007, pages 120–137. http://scitation.aip.org/proceedings/confproceed/963.jsp

243. Orimoto Y, Gu FL, Korchowiec J, Imamura A, Aoki Y (2010) Application of the elongation method to the electronic structure of spin-polarized molecular wire under electric field. Theor Chem Acc 125:493–501

244. Pomogaeva A, Gu FL, Imamura A, Aoki Y (2010) Electronic structures and nonlinear optical properties of supramolecular associations of benzo-2, 1, 3-chalcogendiazoles by the elongation method. Theor Chem Acc 125:453–460