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The Development of Physical & Theoretical Chemistry in Thailand

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ABSTRACT: Theoretical and physical chemistry in Thailand has advanced by leaps and bounds over the past two decades. Many innovative, important developments and applications have earned Thailand a respected, prominent position on the international scientific map. The application of molecular modeling and simulations such quantum mechanics, molecular dynamics and statistical mechanics have been successfully used to investigate the structures and reaction mechanisms of chemical and biological systems, and to design new materials, drugs and chemicals. A valuable resource for researchers is the database, documented and analyzed, which provides comprehensive coverage of the most important research in theoretical and physical chemistry recently conducted in Thailand. A combination of theoretical and experimental methods has been proven to be an effective scientific procedure for reducing the time of product development and for ensuring that a design is right the first time. Cooperative arrangements between universities, national funding agencies and industrial sectors have now become more frequent and more formalized, as industries have found an increasing competitive advantage in forming relationships with universities.

KEYWORDS: Nanotechnology, Theoretical Chemistry, Quantum Chemistry, Molecular Simulations, Molecular Dynamics.

INTRODUCTION

In recent years, numerous innovative developments have occurred in Physical and Theoretical Chemistry, which have led to rapid advancements in the discovery, development, adaptation and modification of materials that are of immense economic and technical benefit to industry.

The Nobel Prize in Chemistry for 1998 was awarded to two theoretical and computational chemists, Walter Kohn for his development of the density-functional theory and John Pople for his development of computational methods in quantum chemistry. Since that auspicious event, computational chemistry and molecular simulations have become vital research tools in scientific and technological development, since they provide important information to help explain and substantiate the observed properties and phenomena, illustrating the apparent changes and reactions at atomic and molecular level. These computational data complement the experimental results and, sometimes, provide information that would be very difficult (or even impossible) to obtain or hard to interpret experimentally. In industrial applications, this knowledge and data can considerably reduce research time, speed up product development, and guide experimentation by providing better understanding and rational, strategic guidelines to problem solving, thus enabling better technical decision-making and ranking of potential chemical structures and formulations in the design and production of pharmaceuticals, chemicals, new materials, and practical nanomaterials.

HISTORICAL DEVELOPMENT OF PHYSICAL & THEORETICAL CHEMISTRY

Improvements in Computational Chemistry have depended on two fundamentals: the development of computational quantum chemistry methodologies, which explain the behaviors of matter and/or molecular materials, and the improvement of computer efficiency to support calculations for large systems[1-4].

Early in 1927, Walter Heitler of Karlsruhe University and Fritz London from München University received Rockefeller scholarships to work on Quantum Mechanics with Erwin Schrödinger at the University of Zurich to study the van der Waals interaction between two hydrogen atoms[1]. This work can be considered as the foundation of the Valence Bond Theory of chemical bonding.

A related development in this field of study, in the years 1926-1927, was the award of a Guggenheim Research Scholarship to Linus Pauling of Caltech to do

postdoctoral research with Professor Arnold Sommerfeld of München University. Influenced by the work of Heitler, Pauling used Quantum Mechanics to study the electronic structure and physical properties of the atomic ion. Concurrently (1927-1928), Robert S. Mulliken of Chicago University received a postdoctoral research grant at Göttingen University. They jointly developed the methodology of the Electronic Structure Theory. In the 1930s, Pauling published papers on the nature of the chemical bond and in 1939 he published his famous textbook, "The Nature of the Chemical Bond", which is one of the most influential chemistry books ever published.

At that time, the applications of the quantum mechanics theory appeared unrealistic, since it could not be applied to any system more complex than the hydrogen atom. Early in 1930, Paul Dirac suggested approximations for the self-consistent field. He showed that if the appropriate approximation method was used, quantum mechanics calculations in large systems could be simplified.

The development of quantum mechanics in the Federal Republic of Germany came to a standstill during the Second World War, as many eminent scientists were forced to flee the country[1]. Consequently, the latter stages of quantum mechanics development took place in the United States, where the key players were Pauling, Mulliken, and Slater. In 1951, Slater proposed the Hartree–Fock–Slater approximation as a simplification of the Hartree–Fock method leading to the first applications to solids in 1952.

John Pople and Walter Kohn, working independently, have been the two most prominent pioneers in Quantum Mechanics. Kohn pioneered the development of the density functional theory. This computational simplification has been further developed and become an essential tool for electronic materials, and atomic and molecular structure[5-7]. Pople pioneered the development of *ab initio* methods and developed one of the most widely used computational chemistry packages. The Gaussian-70 was his first commercial software program released in 1970.

During the past decade, astounding progress has been achieved in the performance of Quantum Mechanics due to both the rapid improvement of computer efficiency and the crucial development of computational quantum chemistry methodologies and algorithms. A wide variety of applications in chemistry, physics, engineering, biology, and computer science have emerged. The theoretical and computational-chemical methods for molecularly based modeling and simulations include:

- Computational quantum chemistry
- Molecular simulations by molecular-dynamics and Monte Carlo methods
- Nanometer-scale modeling of materials
- Materials structure and property correlations (QSARs and QSPRs)
- Information technologies (Chem- and Bio-informatics)

Fundamental Chemistry has now reached the molecular level, more commonly referred to as the nanoscale. Through the use of state-of-the-art spectroscopic techniques and the development of theoretical and computational chemistry, and quantum mechanics, the detailed properties and phenomena at atomic and molecular scales are envisioned. Improvement of material structure is achieved at molecular scales by modifying chemical properties, the amounts of atoms, and atomic orientations in the crystal into the structure of the desired materials. Nowadays, it is an unquestionable fact that computational chemistry has become a well-accepted partner of experimental chemistry.

Theoretical and Computational Chemistry Research Group Founded in Thailand

Even as late as the 1980s, most universities in Thailand had not yet realized the significant impact of the quantum theory to modern chemistry. At that time, research involving quantum chemistry relied mainly on overseas research grants.

With the Alexander von Humboldt Foundation's support, two Thai scientists, Dr. Jumras Limtrakul of Kasetsart University and Dr. Kritsana Sagarik of Ramkhamhaeng University, had the opportunity to conduct postdoctoral research at the Institute of Physical Chemistry, Karlsruhe University. Their work was completed in less than two years (1989-1990) under the intensive academic atmosphere and through their determined dedication.

In 1985, Dr. Jumras Limtrakul founded the Laboratory for Computational and Applied Chemistry, LCAC, in Kasetsart University, with the support of Professor Reinhard Ahlrichs (Director of the Institute of Nanotechnology, Federal Republic of Germany). Initially, the LCAC carried out their main research in Zeolites and Molecular Catalysis[8-13] and later, the research theme was expanded to include molecular drug design, and nanomaterials, and nanobiomaterials. In 2005, the LCAC and collaborative research groups helped to establish the Center of Nanotechnology at Kasetsart University. The Center was recently recognized as the Center of Excellence in Nanoscale Materials Design and Simulation by the National Nanotechnology Center (NANOTEC).

At Chulalongkorn University, Professor Bernd M. Rode, Associate Professor Dr. Sirirat Kokpol, and Professor Dr. Supot Hannongbua founded the

Computational Research Unit, under the support of the Austrian Government. The early research undertaken at Chulalongkorn University related mainly to the Molecular Dynamics of Aqueous Solution and Ion-complexes.

In 2003, Professor Jumras Limtrakul and Professor Supot Hannongbua were awarded the Thailand Outstanding Scientist Award by the Foundation for the Promotion of Science and Technology under the Patronage of H. M. the King for their research in the development and applications of Theoretical and Physical Chemistry to real world problems.

Currently, there is collaboration between Theoretical and Computational Chemistry groups in Thailand to establish research laboratories in universities nationwide. For example, Mahidol University (under the direction of Assistant Professor Yuthana Tantirungrotechai), Suranaree University of Technology (under the direction of Professor Dr. Kritsana Sagarik), Khon Kaen University (under the direction of Associate Professor Dr. Sunantha Hengrasmee), and Prince of Songkhla University (under the direction of Assistant Professor Dr. Pravit Sudkeaw).

This year (2007), NANOTEC recognized the importance of theoretical and computational modeling and simulations and is establishing the Computational Nanoscience Consortium to create a network of nanotechnology researchers in the country, while pooling and utilizing resources for local nanotechnology development. The consortium comprises researchers from nine major universities which conduct nanotechnology research and development. The consortium has worked with the National Electronics and Computer Technology Centre (NECTEC) to set up computing infrastructure and has also worked with the Thai National Grid Centre (TNGC) to utilize TNGC's grid-computing system for high-performance computing.

Master Plans for Chemical Research in Thailand

According to the search results from the Science Citation Index database, the volume of chemical research works from Thailand between 2001-2006 amounted to about 2500 articles, and the number of articles has been increasing every year, as shown in Table 1. If these papers are broadly classified into specific fields of research, the first ten subject categories of science work are as shown in Table 2.

By analyzing this information, the trend in the direction of Thailand's chemical research indicates that the predominant areas are Physical Chemistry, Pharmacology & Pharmacy, Chemical Engineering, Polymer Science, and other fields, respectively. The number of research works in the first ten categories is not significantly different. The relevance of some of these subjects shows Thailand's potential in various branches of chemical research. However, the above subject classification is not totally absolute, since some work may fall into more than one subject area. For example, organic research involved with active natural products can be considered under the subject Pharmacy or Medicinal Chemistry and some physical chemistry research can be categorized into the subject of Multidiscipline Chemistry or Materials Science.

Table 1. International Publications in Chemistry.

Year	Number of research papers
2006	589
2005	516
2004	402
2003	378
2002	342
2001	285

Table 2. Classification of Publications in Chemistry.

No.	Subject Category	Number of research papers	Percent Contribution
1	Physical Chemistry	277	11.03
2	Pharmacology & Pharmacy	264	10.51
3	Chemical Engineering	260	10.35
4	Polymer Science	258	10.27
5	Multidiscipline Chemistry	247	9.83
6	Analytical Chemistry	228	9.08
7	Organic Chemistry	206	8.20
8	Crystallography	205	8.16
9	Medicinal Chemistry	203	8.08
10	Biochemistry & Applied Microbiology	196	7.80

Looking back over the past 5 years, Thailand can proudly claim that the quality of research produced by its physical chemists is acknowledged through presentation in international meetings. Furthermore, much of this research is published in high impact, prestigious academic journals, for example, the *Journal of Physical Chemistry B* (Impact Factor of 4.115), the *Journal of Catalysis* (Impact Factor of 4.533) and *Angewandte Chemie* (Impact Factor 10.232). Also, the works of our researchers are frequently quoted, referred to and applied by international researchers at leading institutes.

Roles and Outputs of Thailand's Theoretical and Computational Chemists

Now, it is possible to classify most of Thailand's theoretical and computational research work according to various topics, as follows:

1. Catalysis
2. Biotechnology
3. Polymer
4. Solution Chemistry
5. Nanoscale Chemistry
6. Cheminformatic Natural Products Library

Theoretical and computational chemical research covers a broad area and involves various branches, such as chemical engineering, polymer, organic chemistry, and pharmaceutical chemistry. This is an encouraging trend because every existing field of chemistry is growing expeditiously. Through the broad spectrum of research and the integration of knowledge through extensive databases, more practical applications may be developed. Physical Chemistry plays a crucial role in elucidating chemical phenomena and their mechanisms, including expounding the quantum properties of matters at the atomic or molecular level. A profound understanding of the basis of the chemical and physical properties of materials serves to further encourage the expansion of applied research.

The majority of physical chemistry research places prominence on the improvement and applications of advanced research methodologies. For example, the electronic embedded QM/MM for the study of complex nanostructural systems – zeolite lattices, nanobiosystem, the improvement of force field functions for macromolecules, the improvement of molecular dynamics for the study of the dynamic properties and orientation within aqueous solutions, the QSAR applications for the design of drugs and chemicals, and data mining accelerating the screening of natural products and potential drugs. As described above, research in physical chemistry tends to employ theories to make use of various subjects, which are all vital to the science and technology.

Industrial Collaboration of Theoretical and Computational Chemistry

Theoretical and Computational Chemistry have achieved an increasingly significant impact on the chemical, pharmaceutical, materials and related industries worldwide. These methods provide valuable tools for obtaining the important properties of systems of interest to these industries. Furthermore, advances in algorithmic and computer hardware have broadened their applications. In the U.S., Europe and Japan, many industries support fundamental work on computational chemistry and materials modeling and simulations, since they:

- Reduce time, waste, and cost to manufacture a product
- Improve quality control
- Reduce time and cost to develop a new product

In Thailand, however, industrial collaboration in theoretical and computational chemistry is very limited. There are still some important limitations in terms of the industrial uses of computational chemistry. To enhance industrial collaboration in theoretical and computational chemistry, several aspects have to be improved:

1. Researchers' expertise: Lack of understanding in theories, analysis, and the output usage, especially in industrial usage.

2. Specific industrial applications which are complex and specialized: Researchers have to determine how to match and incorporate the theories into each operation.

3. Improvement of user-friendly commercial programmes. Even at this time, quantum chemistry user-friendly programmes are widely available. However, there is a need to adapt these for the domestic environment and it is necessary to be able to determine the appropriate methodology.

4. Information and understanding of computational chemistry. Authorized persons responsible should be made aware of the proficiency and versatility of computational chemistry.

However, there are good signs for the future. Some large industrial organizations have realized that for continuing success, they must have the ability to evolve and respond to new technological and societal needs. Therefore, they have increased their investment in research and development. At the same time, the funding agencies, e.g., TRF, NSTDA, have made considerable efforts to encourage industries to become involved in academic research and, at the same time, encourage the academic sector to work closely with related industries. As a result, some collaborative research projects between theoretical and computational chemists and industries have been created. If both the industries and the theoretical and computational chemists continue working together, soon the molecular modeling methods will gain acceptance as practical tools in a variety of industries in Thailand, in the same way that they have been widely accepted internationally.

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