J Multidisciplinary Scientific Journal

MDPI

Editorial

Advance in Molecular Thermodynamics

Fumio Hirata

Theoretical and Computational Molecular Science, Institute for Molecular Science, Okazaki, Aichi 444-8585, Japan; hirata@ims.ac.jp

"Thermodynamics" is one of the oldest but the most fundamental concepts of modern science and technology. The field of science was founded by the giants in science such as Kelvin, Carnot, Planck, etc. The development of the science was originally motivated by the industrial need, or to improve the efficiency of the steam engine. Science is essentially phenomenological and/or macroscopic. Therefore, it is apparently a logical conflict to use the word "Molecular" on "Thermodynamics," because a molecule is a microscopic entity. Nevertheless, the words "Molecular Thermodynamics" seem to have become standard [1]. Therefore, the guest editor put "Molecular Thermodynamics" on the title of the Special Issue in order to feature the recent advances in the field of science.

It is the solvation free energy or the excess chemical potential, and its derivatives with respect to temperature and pressure, that plays crucial roles in chemical processes in solution including those in life phenomena. The equilibrium constant of a chemical reaction is determined by the difference in the chemical potentials between reactant and product. The rate of a chemical reaction is governed essentially by the difference in the chemical potentials between the reactant and the transient state of the chemical species concerned with the reaction. It is important to note that characteristics of molecular species including the electronic structure, molecular structure, etc. are involved in such thermodynamic processes. The molecular recognition process to form a Michaeris–Menten complex in an enzymatic reaction is regulated by the difference in the chemical potentials of the host and guest system before and after the complex formation. A transport process in solution such as the diffusion of a molecule is driven by the gradient of chemical potentials of the species at two different positions in the solution. The stability of a phase in the phase diagram is governed by the chemical potential of each species constituting the phase. A variety of electrochemical processes at the electrode–solution interface are also driven by the chemical potential. Therefore, almost entire spectrum of the molecular science taking place in solution is concerned with the solvation free energy and its derivatives, which are nothing but molecular thermodynamics.

There are several reasons why the field of molecular thermodynamics has been attracting increasing attention. The first of those is the theoretical development in the area of science during last few decades, which is able to reveal in atomistic detail what is going on behind phenomenological thermodynamics. Two typical examples in such a development are the statistical mechanics theory of molecular liquid represented by the RISM/3D-RISM theory and the molecular simulation methods [2,3]. The important feature of those methodologies is to be able to treat the solvent in atomistic detail, which discriminates them from the phenomenological thermodynamics such as the continuum solvent model. The second reason is development of a variety of experimental techniques that reveal microscopic information in molecular detail, which is buried in thermodynamic data. The transient grating technique developed by Terazima and his coworkers and the pressure NMR technique by Akasaka and his coworkers represent the latest developments. The techniques applied to biomolecules in aqueous solution have elucidated not only equilibrium thermodynamics but also the non-equilibrium thermodynamics, or structural fluctuation, that are manifested in the spectroscopic signals [4,5].

Citation: Hirata, F. Advance in Molecular Thermodynamics. *J* **2021**, *4*, 84–85. https://doi.org/10.3390/j4020007

Received: 21 April 2021
Accepted: 21 April 2021
Published: 23 April 2021

There are more practical reasons why molecular thermodynamics is becoming an important field of science. One of those is the demand for drug discovery. Of course, the discovery of a new medicine involves many steps: identifying a target protein or DNA, screening drug candidates, assessing toxicity of the drug candidate, analyzing transportability of the drug candidate among cells, synthesizing the candidate compound, clinical tests, etc. Molecular thermodynamics is concerned with most of those steps except for the clinical test. This is because drugs are nothing but molecules and their function is governed by thermodynamic laws [4,6]. Another practical field in which molecular thermodynamics plays crucial role is electrochemical devices including solar cells, fuel cells, photo-catalysts, and solid-state batteries.

The aim of the Special Issue is to review the advance in molecular thermodynamics during the last few decades, and to explore a new frontier in the field of science.

In this Special Issue, original research articles and reviews are welcome. Research areas may include (but are not limited to) the following: theoretical and experimental physical chemistry, chemical physics, biophysics.

Conflicts of Interest: The author declares no conflict of interest.

References

1. McQuarie, D.A.; Simon, J.D. *Molecular Thermodynamics*; University Science Books: Sausalito, CA, USA, 1999.
2. Hirata, F. (Ed.) *Molecular Theory of Solvation*; Springer Science & Business Media: Berlin, Germany, 2003.
3. Chipot, C.; Pohorille, A. *Calculating Free Energy Differences Using Perturbation Theory*; Free energy calculations; Springer: Berlin, Germany, 2007; pp. 33–75.
4. Terazima, M.; Kataoka, M.; Ueoka, R.; Okamoto, Y. *Molecular Science of Fluctuations toward Biological Functions*; Springer: Berlin, Germany, 2015.
5. Akasaka, K.; Matsuki, H. *High Pressure Bioscience-Basic Concept, Applications and Frontiers*; Springer: Berlin, Germany, 2015.
6. Hirata, F. *Exploring Life Phenomena with Statistical Mechanics of Molecular Liquids*; Apple Academic Press: Palm Bay, FL, USA, 2020.