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Complex molecular systems: a frontier of molecular science

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Remarkable progress has been made in science and technology in the 20th century, and our quality of life has drastically improved compared to that in the previous century. However, due to the rapid increase in the activities of mankind, many resources are now being consumed at an extremely high rate, and an urgent issue in the 21st century is to realize a sustainable society while maintaining our current lifestyle level. In this regard, the current science and technology have begun to show their limitations. Meanwhile, the innovation of life science, which began with the birth of molecular biology, has transformed biology from the natural science that classifies the diverse organisms on Earth to an advanced science for understanding life processes in terms of molecular phenomena. Accordingly, a new view has been formed which considers life as a system consisting of a large number of molecules that realize complex and remarkable functions. This paradigm shift has greatly stimulated molecular science, which has evolved from the understanding of the properties of fundamental molecules through a bottom-up approach. This is because the elemental processes of life are molecular phenomena that achieve ultimate efficiency and specificity at ambient temperatures despite being extremely complicated. In other words, as the ultimate goal of molecular science, it has become important to understand and control the complex molecular systems exhibited by life, with the aim to realize a sustainable society.

Research into complex molecular systems is essentially a study of how to understand and control molecularly multi-body problems. At the same time, there is the question of how to comprehensively elucidate the spatiotemporal behavior of molecular systems spanning a wide time and space scale. For instance, it is important to understand the hierarchical behavior of molecules on the time scales spanning the order of 10^{12}, and to elucidate how a stimulus given over a femtosecond time-scale can lead to a large molecular response in the millisecond or second range. At the same time, it is also essential to clarify how a change in the quantum states of several molecules can lead to the collective motion of a vast number of molecules in the order of 10^{23}. In order to tackle this difficult problem, it has become essential to conduct research of functional analysis and functional control from a variety of aspects that traverse a wide time and space scale.

Until recently, it had been an unrealistic dream to challenge such problems from the forefront, but that opportunity has finally arisen because there has been significant progress in both theoretical and experimental molecular science, which are the two indispensable elements for conducting research on complex molecular systems. In theoretical and computational chemistry for example, due to the advent of huge computational resources, as symbolized by petaflop computers, it has become possible to conduct simulations over periods of milliseconds while tracking the movement of each atom in increments of femtoseconds. In experimental chemistry, on the other hand, it is now possible to track the electrical and structural dynamics of large molecules using ultrafast spectroscopy with a femtosecond time resolution, and to observe the behavior of every single biomacromolecule using single molecule spectroscopy as well as probe microscopy. Furthermore, due to the development of supramolecular chemistry and genetic engineering, it is now possible to create new molecular functions that have never existed before, by controlling or modifying complex molecular systems.

The current problem with this movement in molecular science is that studies taking different approaches tend to proceed separately and have not become a coherent

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movement with the benefit of a bird's-eye view. Therefore, it is critically important to gather the experimental and theoretical research that has been conducted with different backgrounds in order to create more coherent and concerted new fields of science.

In this themed issue, we have collated top-level research that tackles the elucidation of the properties and functions of supramolecules, biomacromolecules and interfaces, which are three prototypical complex molecular systems, through the use of advanced spectroscopy and microscopy, theoretical and computational chemistry, *etc.* We believe that a new direction of molecular science has arisen due to the collaboration of experimental and theoretical research with a broad perspective, which integrates research fields that were regarded as different before.