Editorial

Israel Journal of Chemistry

DOI: 10.1002/ijch.202000052

Special Issue: Protein Simulations – Current State of the Art

The dynamics of proteins is important to all aspects of life, and to many applications where proteins are employed. Whereas the protein structure provides a cue to its function, understanding of proteins and their interactions cannot be complete without understanding their dynamics. Following on protein dynamics by direct measurements is challenging, if at all possible. Computer simulations are often used to bridge the gap between structure and dynamics. The Israeli Nobel Laureates Michael Levitt and Arieh Warshel have been among the pioneers of this field together with Martin Karplus (who won the Nobel Prize on the same occasion), while the theoretical developments from the lab of Shneior Lifson (Laureate of the Israel Prize in Life Sciences) made such studies possible. The *Israel Journal of Chemistry* has dedicated a special issue (Volume 54, Issue 8–9) that focused on computational molecular biophysics in honor of the 2013 Nobel Prize in Chemistry.

The organization known as CECAM (Centre Européen de Calcul Atomique et Moléculaire) was established more than 50 years ago in Paris with the aim of promoting fundamental research on advanced computational methods and their applications. Not surprisingly, many of those applications are in chemistry. The organization has its headquarters in Lausanne. In addition, 17 nodes work with CECAM to organize meetings, events, workshops and schools dedicated to simulations of atoms and molecules. One of these nodes is hosted by the Tel Aviv University; this is the only CECAM node outside of Europe. This Special Issue follows on a CECAM workshop with the same name which took place in Tel Aviv on October 2019 and was funded also by the Israel Science Foundation.

Since the field of protein simulations has started about 40 years ago, it continues to evolve and advance our understanding of complex chemical systems and therefore various aspects in life sciences. Protein simulations constantly strive to approach longer time scales so that they can be directly compared to experimental measurements. Molecular simulations are often motivated to have biological application in understanding the molecular mechanism of diseases. Nonetheless, quantifying the physical chemistry of such complex molecules is still a major challenge to bridge between the microscopic to the macroscopic world. Another major activity in the field is to study more complex systems whose complexity is linked with their function.

The current volume of protein simulations covers the variety of research activities in this field, reflecting its achievement but also its challenges for the coming years. This volume includes ten articles, of which seven are topical reviews and three are original research articles. Subjects that are discussed include theory, best practices, combination of theory and experiment, and specific applications. The cover art for this issue was designed and drawn by Prof. Menachem (Hemi) Gutman, for which we are grateful. We invite the readers to examine the art and the articles and decide for themselves whether or not this Issue can be judged by its cover.

Ran Friedman, Yaakov Levy

Guest Editors