

Computer Simulation of Polymers: Bridging the Gap between Theory and Experiment

In the early history of polymer science, theory and experiment achieved all the milestones. At that time, scientific research was commonly activated by human curiosity or demand to solve a problem. It started with a hypothesis of theory and ended up with the verification of experiment. With the fast expansion of research frontiers, specifically in the typically multi-disciplinary field as polymer science, scientific research was frustrated by too simple theoretical hypothesis or too complicated experimental system. Computer simulation holds the system simpler than experiment. It also allows the hypothesis more complicated than theory. Therefore, it plays the role of bridge to cross over the gap between theory and experiment, as illustrated in Fig. 1 where the common principles and methods of computer simulation addressing various-scale polymer problems are also listed. Current research in polymer science often starts with a hypothesis of theory and ends up with the verification of computer simulation, or it starts with the hypothesis of computer simulation and ends up with the verification of experiment.

The first computer simulation of polymers was performed by Rosenbluth and his wife in 1955, who could ac-

cess the early computer facility in Los Alamos Laboratory and proposed the classic Metropolis sampling algorithm for Monte Carlo simulations in 1953. For computer simulation in chemistry, two Nobel Chemistry Prizes have been awarded separately in 1998 and 2013. Nowadays, along with the rapid development of computer technology, computer simulation has been well accepted in polymer science.

In this year, we celebrate the 40th anniversary of *Chinese Journal of Polymer Science* (CJPS). In this prestige journal, computer simulation of polymers is an important issue. The research groups focusing on computer simulation of polymers have spread over the Mainland of China. They are cultivating young talents who learn both tricks of theory and experiment and can perform computer simulation to solve the polymer problems. In 2010 at Xiamen, Professor Li-Jia An and Professor Yu-Liang Yang organized the first symposium on polymer theory, computation and simulation in the 27th Congress of Chinese Chemical Society. That symposium represented a formation of the community on computer simulations of polymers in China, which later-on greatly enhanced communications among

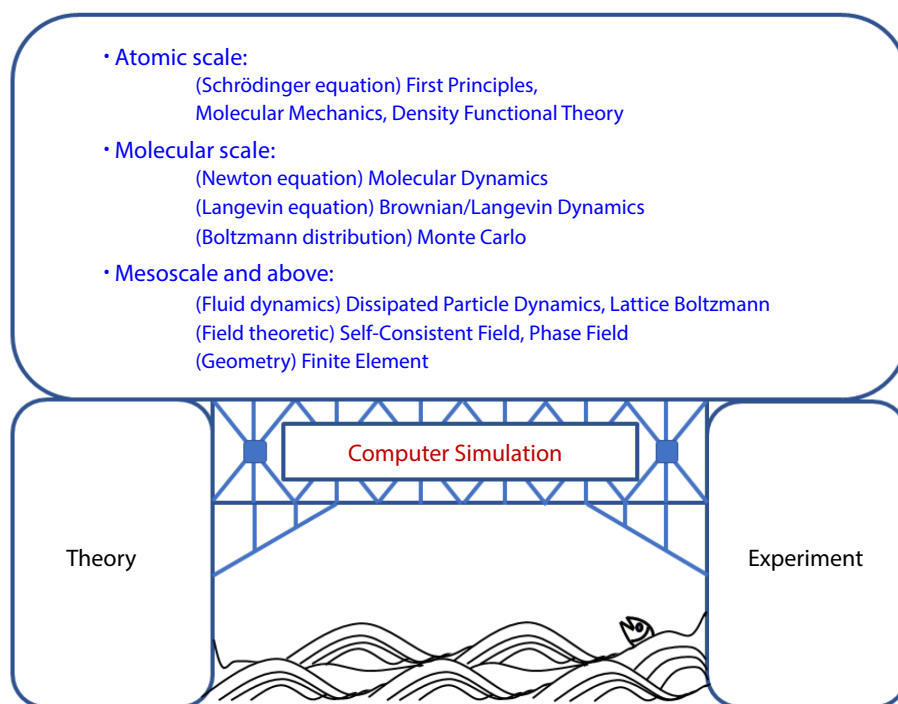


Fig. 1 Illustration of the bridge role of computer simulation in the epistemology of theory and experiment for polymer science. In the above frame, there list various-scale methods and common principles (in brackets) of computer simulation of polymers.

research scientists and students. Since 2012, the annual conferences on polymer theory, computation and simulation have been held around the cities in the mainland of China. Half of this series joined the biennial National Congress of Polymer Science, and another half remained in the scale over 200 participants.

In the coming digital time, computer simulation of polymers will be deeply engaged into those modern movements such as Industry 4.0, Materials Genome Initiative and Artificial Intelligent Technology. It facilitates a visualization and an integration of the fundamental theory in the acceleration of technology innovation for Industry 4.0. It appears as complementary to experiment in the construction of databases for polymer materials genome, as well as in the creation of big data for machine learning of polymer properties. In this promised field, young talents will have ever bright careers.



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The views expressed in this editorial are those of the author.