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PREFACE

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Special Issue: Theory and Simulation of Macromolecules

We are pleased to announce the special issue on Theory and Simulation of Macromolecules published in the *Chinese Journal of Polymer Science*. In recent years, a vibrant research community in the theory and simulation of macromolecules has been established in China [Hu, W. B. Computer simulation of polymers: bridging the gap between theory and experiment, *Chinese J. Polym. Sci.* **2022**, *40*, 709–710], resulting in great progresses in this important area of research in polymer science. We think it is timely to organize a special issue to showcase the activities and achievements of this community. We are thrilled that our call to contribution received enthusiastic response from the community. After peer review, 16 invited contributions are published in this special issue, including 4 Perspectives, 1 Tutorial, 1 Review and 10 Research Articles. These contributions cover a wide range of topics using a variety of techniques including molecular dynamics and Monte Carlo simulations, coarse-grained field theories and machine learning. We believe this special issue gives a snapshot of the research activities on theory and simulation of macromolecules in China, reflecting the breadth and depth of this community.

The Perspective Articles published in this special issue provide summaries of recent progresses and potential future directions in 4 important topics in theory and simulation of macromolecules: (1) Liang-Shun Zhang gave a computational perspective on the design of kinetic pathways to regulate long-range ordered nanostructures self-assembled from macromolecules; (2) Wen-Sheng Xu and Zhao-Yan Sun presented a thermodynamic perspective on the long-standing problem of polymer glass formation; (3) Hai-Xiao Wan, Duo Xu, Xue-Wei Dong, Kai Yang and Li-Tang Yan provided a summary of insights into biophysicochemical principles of Biopolymers obtained *via* theory and simulations; (4) Xu-Ze Zhang, Zhong-Yuan Lu and Hu-Jun Qian offered their perspective on the dynamics properties of polymeric nanocomposites. These perspective articles covered a wide range of topics that are at the forefront of current research in macromolecule science. We believe the publication of this set of Perspectives will motivate further studies in these interest areas of research.

Molecular simulations have become an essential part of modern chemistry and physics. We are pleased to publish a Tutorial article by Duo Xu, Hai-Xiao Wan, Xue-Rong Yao, Juan Li and Li-Tang Yan, "Molecular Simulations in Macromolecular Science", on simulation methods in this special issue. This tutorial provided a useful overview of molecular simulations in the rapid progress of macromolecular science and suggests guidance for researchers who start exploiting molecular simulations in their study. It is our hope that this Tutorial will help readers to initiate new studies using molecular simulations in their research.

Data science and machine learning have been gaining popularity in scientific research in recent years. In their Review, Yun-Qi Li, Ying Jiang, Li-Quan Wang and Jian-Feng Li provided a concise review on the topic of data and machine learning in polymer science, focusing on several recent advances in the description and identification of polymer conformation and structures and the interpretation and prediction of structure-property correlations. This brief review showcases the usefulness of AI and machine learning in polymer science and provides entry point for those interested in the application of these power techniques in their own research.

Moreover, we are pleased to present 10 research articles on Theory and simulation of macromolecules in this special issue, covering various topics ranging from the study of property of single macromolecule and polymer blends, polymer crystallization, and block copolymer self-assembly to dynamic property of multicomponent systems using various methods ranging from molecular dynamics and Monte Carlo simulations, self-consistent field theory to machine learning. This set of research articles provides a snapshot of the activities in theory and simulations of macromolecules.

Finally, we would like to take this opportunity to thank all the authors and reviewers for their valuable contributions and the editors of *Chinese Journal of Polymer Science* for their meticulous editorial effort on this special issue.


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