

Special Topic on AI for Polymers

We are pleased to announce the special topic of “AI for Polymers” published in the *Chinese Journal of Polymer Science* (CJPS). In recent years, the advancements in artificial intelligence (AI) techniques, including machine learning (particularly deep learning) and data-driven modeling, are reshaping how we design, synthesize and characterize polymers. In particular, a strong and lively research community in the development and application of AI techniques to polymer science has emerged in China, making great contributions to this important area of research in polymer science. With the growing interest in the application of AI to polymer science, we believe it is the right time to organize a special topic showcasing the activities and achievements of this community.

We are pleased that our call to contribution received enthusiastic responses. After peer review, 8 invited contributions will be published. Among them, 2 will be published in subsequent issues. These articles cover a range of topics in AI for polymers. We believe this special topic gives a snapshot of the research activities on AI for Polymers in China, reflecting the breadth and depth of this community.

This special topic begins with discussions on AI-driven inverse design of high-performance viscosity modifiers, where Jian Jiang and coworkers present an AI-driven inverse design framework that directly maps target viscosity performance back to optimal molecular structures. In view of challenges due to data scarcity arising from complex chemistries, experimental limitations, and processing-dependent properties, Ying Jiang and coworkers’ review presents some recent advances in data-efficient machine learning for polymers. The cover story of this special topic is contributed by Jiaping Lin and coworkers, where they develop machine-learning-assisted materials genome approach for designing high-performance thermosetting polyimides. In the work of Weihua Li and coworkers, AI-driven automated construction of block copolymer phase diagrams are discussed, demonstrating potential application of AI techniques in fabricating various periodic ordered nanostructures. To evaluate complex correlations among structural variables in the inverse design of polymers, a mean-field approach with the simulated bifurcation algorithm is developed, as elaborated in the work of

Xing-Hua Zhang and coworkers. In the aspect of polymer databases with high-quality, open-source, and large-scale datasets, Ying Wang and coworkers present OpenPoly, a curated experimental polymer database derived from extensive literature mining and manual validation. An interesting application of deep learning is given by Wen-Bin Zhang and coworkers, introducing and demonstrating the efficiency of TmPred, a melting temperature prediction model for thermophilic proteins that combines protein language model, graph convolutional network and Graphormer module. Another interesting application of deep learning is presented by Zhao-Yan Sun and coworkers, describing a machine learning framework based on spatiotemporal point-cloud neural networks to identify and analyze conformational transition pathways of polymer chains.

Written by specialists with various expertise, this special topic provides inspiring examples of the development and application of AI-based models and techniques for polymer science. From the editors’ perspective, we are very pleased and honored to present the approaches, principles, and perspectives in this emerging and important area to our readers. Finally, we would like to express our heartfelt gratitude to all the contributors for their excellent research and time to write up the detailed and pedagogical works, and to the CJPS Editorial Office for their helpful suggestions and excellent coordination of this special topic.



Jian Jiang
Guest Editor



An-Chang Shi
Associate Editor



Li-Tang Yan
Associate Editor

October 2025