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Computational Modeling and Simulations of Polymers

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Message from the Guest Editors

Progress in modelling and simulation is crucial for an improved understanding of polymers. The variety and complexity of polymer structures and systems can only be fully understood with the help of numerical simulations. Nowadays, there are a growing number of problems requiring simulation work. Although lattice, bead-spring or freely jointed bead models are still being used to investigate general features of different types of polymeric systems, more realistic representations are needed in many other instances to understand the properties of specific polymers as well as to explore their potential applications.

This Special Issue offers a broad spectrum of polymer simulations, considering different models and addressing a variety of current interests in terms of systems and applications. Namely, simulation on polymers as drug carriers, compatibilization of polymer mixtures, behaviour of polymer nanostructures under different solvent conditions, physical properties of polymers under stress or physical constrains, formation of the glass state and crystallization and the study of complex systems composed of polymers and nano-objects are included on the list of considered topics.













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Message from the Editor-in-Chief

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