



Computational Modeling of Polymers II

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Message from the Guest Editors

The development of new and innovative polymers is a challenging task. Classical approaches are time and money consuming and should be replaced by computational methodologies that allow the fast and accurate development of innovative materials. Computational modelling has been utilized for alternative approaches and is now indispensable to assist experiments while developing new polymers. In addition, computational methodologies can also help us to study and define the mechanical and physical properties of polymers. In this context, quantum-mechanical calculations, all-atomistic and coarse-grained molecular dynamics simulations, and elastic network models have become a powerful tool for analysing complex physical phenomena, i.e., bond vibrations, diffusion, and rheology of polymeric materials. The main aim of this Special Issue is to investigate more recent computational approaches used to develop and study polymers. This Special Issue will provide an opportunity for scientists, engineers, and practitioners to present their more relevant studies and findings in this area.





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