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Computational Modeling of Polymers

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Deadline for manuscript submissions:
closed (20 April 2022)

Message from the Guest Editors

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 a fast and accurate development of innovative materials. Computational modelling has been emerging as alternative approaches and nowadays is indispensable to assist experiments while developing new polymers. In addition, computational methodologies can also help to study and defining mechanical and physical properties of polymers. In this contests, 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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Message from the Editor-in-Chief

Since its foundation in 2009, *Polymers* has developed into an internationally renowned, extremely successful open access journal. The editorial team and the editorial board dedicatedly combine open-access publishing and high-quality rigorous peer reviewing. The performance of the journal has proven this strategy to be well-suited and highly successful. This is reflected in the increasing impact factor of *Polymers*, the most recent one being 5.0.

I would like to invite you to contribute to the success of the journal by sending us your high quality research papers. We would be pleased to welcome you as one of our authors.

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