# Special Issue

# Computational Modeling of Polymers

### 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.

### Guest Editors


Dr. Riccardo Concu

Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, 4169-007 Porto, Portugal

Dr. Michael González-Durruthy

Science and Technology Park, University of Porto, 4169-007 Porto, Portugal


### Deadline for manuscript submissions

closed (20 April 2022)


## Polymers

an Open Access Journal by MDPI

Impact Factor 4.9
CiteScore 9.7
Indexed in PubMed

mdpi.com/si/84583

*Polymers*
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
polymers@mdpi.com

mdpi.com/journal/polymers

# Polymers

an Open Access Journal by MDPI

Impact Factor 4.9
CiteScore 9.7
Indexed in PubMed

mdpi.com/journal/polymers

# About the Journal

## 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 4.9.

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.

## Editor-in-Chief

Prof. Dr. Alexander Böker
Fraunhofer-Institut für Angewandte Polymerforschung, Lehrstuhl für Polymermaterialien und Polymertechnologie, Universität Potsdam, Geiselbergstraße 69, 14476 Potsdam-Golm, Germany

## Author Benefits

**Open Access:**

free for readers, with article processing charges (APC) paid by authors or their institutions.

**High Visibility:**

indexed within Scopus, SCIE (Web of Science), Ei Compendex, PubMed, PMC, FSTA, CAPlus / SciFinder, Inspec, and other databases.

**Journal Rank:**

JCR - Q1 (Polymer Science) / CiteScore - Q1 (General Chemistry )