

## Special Issue

# Modeling and Simulations of Smart and Responsive Polymers

### Message from the Guest Editors

Smart or responsive polymers are soft materials that display controllable property changes in response to an applied physical, chemical, or biological stimulus. In most cases of practical interest, the functionality of such materials can be modulated with the inclusion of responsive chemical groups and solvents, co-polymerization, conjugation with nanoparticles, proteins, and various other methods. For the discovery, design, and optimization of smart polymers for future applications, it is essential to gain a fundamental understanding of their dynamic structure/stimulus/property relationships through theory, modeling, and simulations.

This Special Issue welcomes contributions drawing on the cutting-edge theory and computational modeling of stimulus responses in smart polymers. Given the importance of responsive behavior at varied length- and time-scales, we welcome research involving (but not limited to): (1) phenomenological and constitutive models, (2) all-atom molecular dynamics (MD), (3) coarse-grained MD, (4) quantum chemical modeling, (5) continuum-level simulations, and (6) structure–property correlation models.

### Guest Editors

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### Deadline for manuscript submissions

closed (20 May 2024)



## Polymers

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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 4.7.

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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### Editor-in-Chief

Prof. Dr. Alexander Böker

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