# Special Issue

## Modelling and Simulations in Polymer Surface Chemistry

### Message from the Guest Editors

This Special Issue focuses on theoretical models and computational studies of polymers' surfaces and interfaces. The surfaces of polymers and composites are of critical importance for numerous technological applications: sensors, electrochemistry, coating, energy and biological applications, etc. It is an intrinsically multidisciplinary area where chemical and material syntheses are in close contact with nanotechnology, theoretical chemistry and physics.Papers are sought that relevance to this field, focusing on modelling, theoretical and computational work, with or without supporting experimental results.The scope of this Special Issue is wide and we are looking forward to receive contributions on simulations of characterization techniques or models of functionalization of polymers' surfaces, as well as theoretical approaches that suggest the novel application of polymers' surfaces in fields including electrochemistry, catalysis, coating and corrosion protection, drugs delivery, sensing and photochemistry. Simulations of self-healing polymers and polymers' degradation are also relevant when they specifically address the role of interfaces and surfaces.

### Guest Editors

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### Deadline for manuscript submissions

closed (20 February 2022)

**Polymers**

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**Impact Factor 4.7**
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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.

## Editor-in-Chief

Prof. Dr. Alexander Böker
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