# Special Issue

# New Insight into Polymer Dynamics

## Message from the Guest Editor

Molecular configuration, electronic properties (electronic-states) and thermodynamic properties of polymeric molecules establish foundations for the various macroscopic properties of polymer materials. Non-bonding interactions, aggregation states and the energy (potential energy and kinetic energy) evolution of polymer molecular chains in polymer materials account for the intrinsic mechanism behind material physical characteristics such as thermal stability, phase transition, and electrical or mechanical strength. The first-principle calculations and molecular dynamics simulations are capable of building up molecular-level models for polymer-based materials in order to evaluate and predict their electrical, thermal and mechanical properties, whilst elucidating molecular-scale mechanisms and regulating the relationship between micro-structure and macro-properties to lay theoretical foundations for the optimization and design of advanced and applicable polymer-hosted composites. The purpose of this Special Issue is to report the latest research achievements on polymer modification or design through theoretical calculations or molecular dynamics simulations.

## Guest Editor

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## Deadline for manuscript submissions

closed (31 December 2024)

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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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