Special Issue

Simulation and Calculation of Polymer Composite Materials

Message from the Guest Editors

Dear Colleague,

Polymeric solids exhibit a complex structure–property relationship. By adding extra phases into the polymeric matrix, significantly enhances the tunability of their properties but renders their rational design even harder. Physics- and data-driven modelingoffer an attractive opportunity to revisit these challenges facing polymer composite design.

In this Special Issue, we invite contributions that address several aspects pertaining to the modelling and inverse design of polymer composites, including those that decipher the structure–property relationship of polymeric solids by conventional modeling tools, develop new simulation schemes to predict polymer properties by simplifying the underlying physics, build surrogate simulation engines of polymer composites by machine learning, and combine high-throughput simulations and machine learning to accelerate the discovery of novel polymer materials. Any original contributions (including reviews) relevant to rationalizing computational modeling of polymer composites and their inverse design are welcome. We hope that this Special Issue will modestly help to stimulate new developments in that direction.

Guest Editors

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Deadline for manuscript submissions

closed (5 May 2025)

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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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