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Research on Polymer Simulation, Modeling and Computation

Guest Editors:

Dr. Shengfeng Cheng

Dr. Jiajia Zhou

Dr. Ting Ge

Deadline for manuscript submissions:
closed (30 October 2023)

Message from the Guest Editors

In silico simulation, modeling, and computation have evolved into powerful tools to reveal the molecular mechanisms underlying the macroscopic phenomena and behavior of polymers, predict their physicochemical properties, and discover and design next-generation polymeric materials. A wide range of simulation methods and packages, from those based on quantum mechanics with subatomic resolutions to continuum frameworks dealing with bulk materials, are at the disposal of researchers to study polymers over a full spectrum of length, time, and energy scales under various conditions. Multiscale models are also in rapid development and validation. This Special Issue aims to serve as a platform to allow polymer researchers to exchange exciting results, recent progress, and emerging ideas on understanding polymers from the perspectives of simulation, modeling, and computation. The issue welcomes reports and reviews covering any aspect of polymer modeling, using methods including but not limited to density functional theory, molecular dynamics simulation, coarse-grained modeling, lattice Boltzmann simulation, self-consistent field theory, multiscale simulation.

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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 5.0.

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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