Multiscale Modeling and Simulation of Polymer-Based Composites

Guest Editors:

Dr. Maoyuan Li
State Key Laboratory of Material Processing and Die & Mold Technology, Huazhong University of Science and Technology, Wuhan 430074, China

Prof. Dr. Yun Zhang
State Key Laboratory of Material Processing and Die & Mold Technology, Huazhong University of Science and Technology, Wuhan 430074, China

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Message from the Guest Editors

Dear Colleagues,

The structure of polymers and their composites is hierarchical and rich. It is a complex multiscale system with characteristic sizes, from nanometers to millimeters, and characteristic times, from femtoseconds to seconds. Thus, multiscale modeling and simulation methods, including density functional theory, molecular dynamics, Brownian dynamics, dissipative particle dynamics, the lattice Boltzmann method, Monte Carlo, computational fluid dynamics, and the finite element method, are the key to understand the complex behavior and various phy-chemical properties of polymers and their composites. The aim of this Special Issue is to highlight progress in the multiscale modeling and simulation methods of polymers and their composites. Any reports and reviews covering the aspects of multiscale modeling and simulations are welcome, using methods including, but not limited to, those mentioned above.

Keywords:

- polymer
- polymer-based composite
- computational modeling
- molecular dynamics
- computational fluid dynamics
- finite element method

Special Issue

Editor-in-Chief

Prof. Dr. Alexander Böker
Lehrstuhl für Polymermaterialien
und Polymertechnologie,
University of Potsdam, 14476
Potsdam-Golm, Germany

Message from the Editor-in-Chief

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