



Multiscale Modeling and Simulation of Polymer-Based Composites

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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 physicochemical 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





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