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# Multi-Scale Modeling of Polymer-Based Nanocomposites

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**closed (20 July 2022)**

## Message from the Guest Editors

Dear Colleagues,

Polymer nanocomposites attract widespread attention from researchers. Computational simulation has unique advantages in establishing the relationship among the microscopic structure, the thermodynamic mechanisms, and the properties. The important properties include the nanocomposite rupture mechanism, viscoelasticity, rheology, electrical conductivity, thermal conductivity, formation kinetics, and so on. These properties depend on various factors, such as the polymer–nanoparticle interaction; the size, shape and concentration of nanoparticles; the physical and chemical properties of the polymer and nanoparticles and so on. Therefore, it is very important to investigate the underlying mechanisms at the molecular/microscopic scale, and to provide an understanding bridging between the mechanisms at microscopic scale and properties at macroscopic scale. Computational methods including but not limited to molecular dynamics simulation, Monte Carlo simulation, mean-field theory, classical density functional theory, and the finite element method are all suitable in this Special Issue.

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## Message from the Editor-in-Chief

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