Special Issue

Multi-Scale Modeling of Polymer-Based Nanocomposites

Message from the Guest Editors

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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Materials (ISSN 1996-1944) was launched in 2008. The journal covers twenty-five comprehensive topics: biomaterials, energy materials, advanced composites, advanced materials characterization, porous materials, manufacturing processes and systems, advanced nanomaterials and nanotechnology, smart materials, thin films and interfaces, catalytic materials, carbon materials, materials chemistry, materials physics, optics and photonics, corrosion, construction and building materials, materials simulation and design, electronic materials, advanced and functional ceramics and glasses, metals and alloys, soft matter, polymeric materials, quantum materials, mechanics of materials, green materials, general. *Materials* provides a unique opportunity to contribute high quality articles and to take advantage of its large readership.

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