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Study on the Mechanical Behavior and Molecular Dynamics of Functional Polymer Structures

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Deadline for manuscript submissions:
closed (10 December 2021)

Message from the Guest Editor

Thanks to the rapid development and expansion of computational resources in the past 20 years, we have been able to extend the depth of our gaze on nature and engineering to the microscopic world at the atomic level through computer simulation. In particular, research exploring the macromolecular properties of materials as well as the molecular mechanics of intrinsic microstructures has been spotlighted for polymer nanocomposites in which functional polymers and/or nanoparticles are inserted.

The main goal of this Special Issue is to collect the latest contributions to research topics on functional polymers and polymer-based nanostructures. We welcome all kinds of computational/theoretical approaches, such as continuum mechanics of composites, all-atom molecular dynamics, density functional theory, Monte-Carlo method and coarse-grained modeling. Furthermore, multi-scale modeling that combines two or more simulation methodologies, coupling computer simulation with experiments and new polymer material design studies through machine learning algorithms are also highly recommended.

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Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

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