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New Insight into Polymer Dynamics

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Message from the Guest Editor

Molecular configuration, electronic properties (electronic-states) and thermodynamic properties of polymeric molecules establish foundations for the various macroscopic properties of polymer materials. Non-bonding interactions, aggregation states and the energy (potential energy and kinetic energy) evolution of polymer molecular chains in polymer materials account for the intrinsic mechanism behind material physical characteristics such as thermal stability, phase transition, and electrical or mechanical strength. The first-principle calculations and molecular dynamics simulations are capable of building up molecular-level models for polymer-based materials in order to evaluate and predict their electrical, thermal and mechanical properties, whilst elucidating molecular-scale mechanisms and regulating the relationship between micro-structure and macro-properties to lay theoretical foundations for the optimization and design of advanced and applicable polymer-hosted composites.

The purpose of this Special Issue is to report the latest research achievements on polymer modification or design through theoretical calculations or molecular dynamics simulations.

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Message from the Editor-in-Chief

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