Special Issue

Research in Molecular Dynamics Simulation of Polymers

Message from the Guest Editor

Simulation studies of polymers that use models at various scales of length and time are coming to play an increasingly vital role in advancing physicochemical insights into the polymer materials. Quantum potentials, force fields, coarse-grained models, mean field method, continuum-level modeling and, more recently, machine learning-driven simulation provide the solutions to tackle challenging problems via a simulation approach. Nevertheless, there are certain knowledge gaps between the development of high-resolution models and their deployment for appropriate research projects. This Special Issue of *Crystals* aims to cover: (i) development and deployment of simulations models for study of polymer in general; (ii) analysis and computation of desirable physical, chemical and electrochemical properties of polymers; (iii) informatics of polymers and transfer learning for the discovery of novel materials structures, properties and applications; (iv) guidance for the design of polymer and benefits for design of experiments.

Guest Editor

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Message from the Editor-in-Chief

Welcome to *Crystals*, the journal dedicated to the fascinating world of crystallographic research! Crystals are more than mere decorative elements; they hold the key to understanding the fundamental structure of matter. Our mission is to explore the crucial significance of this research across various fields. From medicine to technology, chemistry to geology, crystals play a vital role. Their structure provides insights into new advanced materials, innovative drugs, and groundbreaking technologies. Through *Crystals*, we delve into the microscopic world to discover solutions that will shape the future. Join us on a journey through the *Crystals*, where science merges with beauty and innovation.

Editor-in-Chief

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