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Molecular Dynamics Simulations of Polymers

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Message from the Guest Editor

Polymers are macromolecules with a large variety of chemical structures and morphologies which determine their unique and various properties. They are widely used in many different areas, from medicine to the aerospace industry. Understanding polymers' interactions and morphology on the atomistic scale is of paramount importance to interpret and improve their properties. In recent years, molecular dynamics simulations have become a standard tool alongside experiments to understand the morphology of polymers on the atomistic scale. Often, molecular dynamics brings valuable information to interpret experimental data.

This Special Issue aims to collect scientific articles and reviews from various topics related to molecular dynamics simulations of polymers, such as morphology, mechanical properties, phase behavior, and optical and electrical properties, to name a few. Both atomistic and coarsegrained molecular dynamics contributions are welcome. In addition, synthetic as well as natural polymer-related research will be considered. We hope that this Special Issue can further help to promote the use of molecular dynamics simulations in contemporary polymer research.













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Editor-in-Chief

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Message from the Editor-in-Chief

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