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## First Principles Calculations and Molecular Dynamics Simulations in Polymer Research

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### Message from the Guest Editor

First-principles calculations and molecular dynamics simulations have been emerging as the most powerful and efficient tools for providing a scientific understanding to elucidate experimentally observed phenomena and offering alternative ways for materials characterization, design and property prediction. With the help of first-principles calculations, more accurate descriptions of the interactions between the atoms can be obtained for polymers themselves, as well as their interactions with other species at the electron level, which is significant for the investigation of electrical, thermal and chemical properties, such as electrical conductivity and chemical adsorption. Molecular dynamics simulations, on the other hand, are helpful in obtaining detailed information regarding the interactions and deformations of polymer chains at the atomic level when exposed to external mechanical or thermal loadings.



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