Special Issue

First Principles Calculations and Molecular Dynamics Simulations in Polymer Research

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 spices at the electron level, which is significant for the investigation of electrical, thermal and chemical properties, such as electrical conductivity and chemcial adsorption. Molecular dynamics simulations, on the other hand, are helpful in obtaining detailed information regarding the interactions and deformations of polymer chains at the atomtic level when exposed to external mechanical or thermal loadings.

Guest Editor

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Since its foundation in 2009, *Polymers* has developed into an internationally renowned, extremely successful open access journal. The editorial team and the editorial board dedicatedly combine open-access publishing and high-quality rigorous peer reviewing. The performance of the journal has proven this strategy to be well-suited and highly successful. This is reflected in the increasing impact factor of *Polymers*, the most recent one being 4.7.

I would like to invite you to contribute to the success of the journal by sending us your high quality research papers. We would be pleased to welcome you as one of our authors.

Editor-in-Chief

Prof. Dr. Alexander Böker
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