Special Issue

Recent Advances in the Design and Molecular Dynamics Simulations of Polymeric Materials

Message from the Guest Editors

The structural determination of polymeric materials is often hampered by its inner complexity, featuring large segments of amorphous organization, interspersed by areas of crystallized materials of variable sizes. Such inner disorganization makes it extremely complicated to comprehend their molecular structure and hinders the design of new polymeric materials of advanced applications. Molecular simulations arise as a powerful alternative tool to understand, at the atomistic level the physic-chemical basis that determine those properties that will encompass their practical use. In this Special Issue, we present the latest advances in using simulations to characterize the organization of such materials, the main aim being to demonstrate how the combination of experimental information with the simulations of polymeric systems allows one to increase the understanding and development of new advanced materials of better applicability in fields such as nanotechnology, biomedicine or pharmaceutics. Not only does this Special Issue focus on what Molecular Dynamics can contribute, but also in the combination of the technique with others that belong to the field of Computational Chemistry.

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Message from the Editor-in-Chief

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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