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

Guest Editors:

Dr. David Zanuy
Department of Chemical Engineering (EQ), Universitat Politècnica de Catalunya (UPC), Barcelona, Spain

Dr. Guillem Revilla-López
DC Technology & Corporate Venturing, Agustín de Betancourt s/n, 28935 Móstoles, Madrid, Spain

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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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Editor-in-Chief

Prof. Dr. Alexander Böker
Lehrstuhl für Polymermaterialien und Polymertechnologie, University of Potsdam, 14476 Potsdam-Golm, Germany

Message from the Editor-in-Chief

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Contact Us

Polymers Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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