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Molecular Simulations for Structure-Property Relationships in Novel Polymeric Materials

Guest Editor:

Dr. Baris Demir
Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Cnr College Rd & Cooper Rd, Brisbane 4072, Australia

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Message from the Guest Editor

Due to the depletion of fossil resources and hence the rising price, and environmental problems, new novel monomers need to be designed and tested to replace bisphenol derivatives that are toxic and environmentally unfriendly.

Using novel polymers has imparted multifunctionality to composite materials. Novel polymer composites combine properties such as ionic conductivity, thermal conductivity and hydrophilicity in addition to promising thermo-mechanical properties. For example, interpenetrating polymer networks (IPNs) that are defined as a combination of at least two polymers that form a network can be promising host matrix for polymer composites because each network component will impart different properties or contribute to multiple properties of the resultant composite.

The aim of this Special Issue is to highlight the importance of using molecular simulation techniques in modelling, testing and tuning novel and/or bio-based polymeric materials and their composites for various applications in the aerospace, automotive and energy industries.

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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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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.

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Contact Us

Polymers Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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