polymers

IMPACT FACTOR 4.7 | Indexed in: PubMed | CITESCORE 8.0

an Open Access Journal by MDPI

Modelling and Simulation of Proteins, Biopolymers and Biocompatible Materials

Guest Editors:

Dr. Tarsila Gabriel Castro
1. Centre of Biological Engineering, Campus de Gualtar, University of Minho, 4710-057 Braga, Portugal
2. LABBELS–Associate Laboratory, Braga/Guimarães, Portugal

Dr. Cristina E. A. Sousa
BioMark Sensor Research-School of Engineering of the Polytechnic Institute of Porto, Rua Dr. António Bernardino de Almeida, 431, 4249-015 Porto, Portugal

Dr. Carla Silva
Centre of Biological Engineering, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal

Deadline for manuscript submissions:
closed (30 April 2024)

Message from the Guest Editors

Dear Colleagues,

Today, molecular modelling techniques comprise valuable methods and tools assisting a wide area of knowledge and experiments, both guiding and explaining molecular processes. This Special Issue focuses on the modelling and simulation of biopolymers and biomaterials which represent a breakthrough in the field in terms of describing important biological processes or applications.

Potential topics include (but are not limited to) the following:

- Protein folding and stability;
- Peptidomimetics design;
- Functional materials;
- Quantum calculations for biopolymers;
- Docking in DNA or in proteins/enzymes;
- Molecular Dynamics Simulations of proteins and biomaterials;
- MD simulations to estimate physicochemical and rheological properties;
- Deep Eutectic mixtures as solvents for chemical reactions;
- Modelling of Deep Eutectic mixtures.

We hope that this Special Issue can help to promote the use of molecular modelling methods in contemporary research by offering a fresh perspective on its use in biopolymers.

mdpi.com/si/139679

polymers

IMPACT FACTOR 4.7 | Indexed in: PubMed | CITESCORE 8.0

an Open Access Journal by MDPI

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

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 5.0.

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.

Author Benefits

Open Access: free for readers, with article processing charges (APC) paid by authors or their institutions.
High Visibility: indexed within Scopus, SCIE (Web of Science), Ei Compendex, PubMed, PMC, FSTA, CAPlus / SciFinder, Inspec, and other databases.
Journal Rank: JCR - Q1 (Polymer Science) / CiteScore - Q1 (General Chemistry)

Contact Us

Polymers Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/polymers
polymers@mdpi.com
𝕏@Polymers_MDPI