materials

IMPACT FACTOR 3.4

Indexed in: PubMed

CITESCORE 5.2

an Open Access Journal by MDPI

Computational Modeling and Simulation of Polymers and Biopolymers

Guest Editors:

Dr. Petra Bačová

Dr. Laurence G. D. Hawke

Dr. Constantinos Simserides

Deadline for manuscript submissions:
10 June 2024

Message from the Guest Editors

Computational approaches represent a sustainable alternative to costly experimental techniques. Concerning polymer simulations, systematic hierarchical approaches are highly valued as they provide a quantitative description across the scales. These approaches also contribute to the progress of polymer informatics and new tools such as machine learning algorithms by unifying data from various simulation techniques while simultaneously verifying and extending them by an iterative loop with up-to-date experimental results. The theoretical study of soft matter is complimented by computational modelling, which is commonly based on mean-field approximations. Among several other topics, the equilibrium molecular self-assembly of block copolymers, the linear and nonlinear rheological properties of entangled polymer chains under shear, and the industrial processing of polymeric matter are often studied by mean-field computations.

In this Special Issue, we would like to welcome all contributions including, but not limited to, the following topics:

Molecular dynamics and Monte Carlo simulations;
Polymer informatics;
Atomistic simulations;
Coarse-grained methods;
Molecular rheology.

materials

IMPACT FACTOR 3.4 | Indexed in: PubMed | CITESCORE 5.2

an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Maryam Tabrizian
1. Department of Biomedical Engineering, Faculty of Medicine and Health Sciences, McGill University, Montreal, QC H3A 2B6, Canada
2. Faculty of Dentistry and Oral Health Sciences, McGill University, 3640 Rue University, Montreal, QC H3A 0C7, Canada

Message from the Editor-in-Chief

Materials (ISSN 1996-1944) was launched in 2008. The journal covers twenty-five comprehensive topics: biomaterials, energy materials, advanced composites, advanced materials characterization, porous materials, manufacturing processes and systems, advanced nanomaterials and nanotechnology, smart materials, thin films and interfaces, catalytic materials, carbon materials, materials chemistry, materials physics, optics and photonics, corrosion, construction and building materials, materials simulation and design, electronic materials, advanced and functional ceramics and glasses, metals and alloys, soft matter, polymeric materials, quantum materials, mechanics of materials, green materials, general. *Materials* provides a unique opportunity to contribute high quality articles and to take advantage of its large readership.

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), PubMed, PMC, Ei Compendex, CaPlus / SciFinder, Inspec, Astrophysics Data System, and other databases.
Journal Rank: JCR - Q2 (*Metallurgy & Metallurgical Engineering*) / CiteScore - Q2 (*Condensed Matter Physics*)

Contact Us

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

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

mdpi.com/journal/materials
materials@mdpi.com
𝕏@Materials_Mdpi