entropy

an Open Access Journal by MDPI

IMPACT FACTOR 2.1

Indexed in: PubMed

CITESCORE 4.9

Molecular Dynamics Simulations of Biomolecules

Guest Editors:

Dr. Donald J. Jacobs
Department of Physics and Optical Science, University of North Carolina at Charlotte, 9201 University City Blvd., Charlotte, NC 28223, USA

Dr. Amar Singh
Center for Computational Biology, The University of Kansas, Lawrence, KS 66047, USA

Deadline for manuscript submissions:
closed (30 June 2023)

Message from the Guest Editors

Molecular dynamics (MD) computational studies have played a critical role in both detailed atomic-scale and coarse-grained level information of a physical system. The MD simulation techniques have established their relevance in modern drug development processes, all-atom simulations of protein folding, protein–ligand docking, and mechanisms of large biomolecular networks. With remarkable advances in computing hardware and theoretical advancement, it is now possible to run longer MD simulations and thus a highly promising future of MD simulations.

The aim of this Special Issue is to present recent applications of MD simulations in life sciences, especially in the context of interactions and free energy landscapes. This Special Issue is open to researchers working with MD simulations at any of these levels: a) thermodynamics, b) dynamics, and c) structural or conformational transitions. Original research papers and review articles that address the MD simulations of biomolecules are all welcome.

entropy

IMPACT FACTOR 2.1 | Indexed in: PubMed | CITESCORE 4.9

an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Kevin H. Knuth
Department of Physics, University at Albany, 1400 Washington Avenue, Albany, NY 12222, USA

Message from the Editor-in-Chief

The concept of entropy is traditionally a quantity in physics that has to do with temperature. However, it is now clear that entropy is deeply related to information theory and the process of inference. As such, entropic techniques have found broad application in the sciences.

Entropy is an online open access journal providing an advanced forum for the development and/or application of entropic and information-theoretic studies in a wide variety of applications. *Entropy* is inviting innovative and insightful contributions. Please consider *Entropy* as an exceptional home for your manuscript.

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), Inspec, PubMed, PMC, Astrophysics Data System, and other databases.
Journal Rank: JCR - Q2 (*Physics, Multidisciplinary*) / CiteScore - Q1 (Mathematical Physics)

Contact Us

Entropy Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

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

mdpi.com/journal/entropy
entropy@mdpi.com
𝕏@Entropy_MDPI