



entropy



an Open Access Journal by MDPI

Molecular Dynamics Simulations of Biomolecules

Guest Editors:

Message from the 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)

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.



mdpi.com/si/100248

Special Issue



entropy



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, St. Alban-Anlage 66
4052 Basel, Switzerland

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

mdpi.com/journal/entropy
entropy@mdpi.com
[X@Entropy_MDPI](#)