



an Open Access Journal by MDPI

Molecular Simulations of Functionalized Nanoscale Materials

Guest Editors:

Dr. Paul Mulheran

Department of Chemical and
Process Engineering, University
of Strathclyde, Glasgow G1 1XJ,
UK

Dr. Giorgia Brancolini

Consiglio Nazionale delle
Ricerche, CNR NANO - Institute
Nanoscience, Center S3, via G.
Campi 213/A, 41125 Modena,
Italy

Deadline for manuscript
submissions:

closed (30 April 2022)

Message from the Guest Editors

Dear Colleagues,

Well-designed molecular simulations can give atomistic insight into the interactions between a biomolecule and an inorganic/organic surface, revealing details that cannot be accessed through experiment alone. In turn, experiments can validate some key aspects of the simulation to build confidence in the theoretical predictions. This synergy between experiment and simulation can be harnessed to optimize the design of functionalized nanoscale systems, and indeed provide rational design tools to create new technologies.

In this Issue, we bring together research at the interface between modelling and experiment, where molecular simulation plays an important role in the scientific discovery and development of functionalized nanoscale materials. The systems of interest include, amongst others: Targeted drug delivery; Novel therapeutics and vaccines; Imaging and diagnostics; Biosensors; Industrial catalysis.

Full papers and short communications covering methodological and theoretical aspects, as well as interdisciplinary approaches underlying the potential interpretation of experimental data and applications are all welcome.

Dr. Paul Mulheran
Dr. Giorgia Brancolini



mdpi.com/si/61700

Special Issue



an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Maurizio Battino

Department of
Odontostomatologic and
Specialized Clinical Sciences,
Sez-Biochimica, Faculty of
Medicine, Università Politecnica
delle Marche, Via Ranieri 65,
60100 Ancona, Italy

Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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, MEDLINE, Embase, CAPlus / SciFinder, and other databases.

Journal Rank: JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Inorganic Chemistry)

Contact Us

*International Journal of Molecular
Sciences* Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

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

mdpi.com/journal/ijms
ijms@mdpi.com
X@IJMS_MDPI