

Special Issue

Molecular Simulations of Functionalized Nanoscale Materials

Message from the Guest Editors

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.

Guest Editors

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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.

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