

Special Issue

Research on Molecular Dynamics

Message from the Guest Editors

Molecular dynamics (MD) simulation has emerged as a fundamental research methodology in biology, material sciences, and chemical physics. Many advanced tools, including cryo-electron microscopy, X-ray crystallography, solid-state nuclear magnetic resonance, and fiber diffraction, have been developed to determine molecular structure and function. Recent advances in the computational platform, algorithms, analysis tools, software, and high-performance computing have made molecular simulations useful for investigating more complicated and large systems.

We warmly welcome your contributions to this Special Issue on “Research on Molecular Dynamics.” This Special Issue will cover any aspect of MD simulation, including the theory, techniques, and computational or methodological developments for the result analysis. Original research papers and review articles addressing MD simulation applications to diverse biomolecular systems, interactions, and functions are welcome. Submission of combined simulation and experimental studies is also encouraged.

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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