Special Issue

Recent Progress in Advanced Computing Techniques for Molecules and Nanomaterials

Message from the Guest Editor

Recent developments in advanced computing techniques have significantly contributed to the design and property prediction of materials at the molecular and nanoscale levels. For example, machine learning (ML) and artificial intelligence (AI)-based methodologies play a key role in efficiently modeling complex physical and chemical interactions by processing large datasets. In particular, studies combining molecular dynamics (MD) simulations with hybrid modeling techniques are contributing to the in-depth analysis of the mechanisms underlying nanomaterials. In nanomaterials research, computing techniques have been applied to predict the electrochemical and optical properties of materials such as quantum dots, nanotubes, and graphene and its derivatives. This has led to groundbreaking developments in applications ranging from energy storage and catalysis to sensor technologies. This Special Issue highlights the progress and applications of advanced computational technologies in the field of computational chemistry and nanomaterials, offering insights into future research directions.

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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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