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Molecular Dynamics Simulations

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Message from the Guest Editors

Dear Colleagues,

Molecular Dynamics (MD) simulations, nowadays, allow to explore time-dependent changes occurring in molecular systems thus providing paramount information to understand a wide range of chemical and biological phenomena. In many cases, MD can be viewed as a counterpart to experiment as MD data frequently help interpret *in vivo* and *in vitro* results and are invaluable in proposing hypotheses and experiments.

This Special Issue on “Molecular Dynamics Simulations” is open to researchers working with Molecular Dynamics at any level. Papers addressing methodological or computational developments on force field effects, full-atom/coarse grained calculations, explicit/implicit treatment of solvent, analyses of trajectories, etc., as well as papers reporting applications to diverse molecular systems, interactions, protein function, etc., are welcome. Submission of up-to-date review articles is also encouraged.

Prof. Dr. Luis F. Pacios
Dr. María Garrido-Arandia
Guest Editors



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Special *Issue*



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Message from the Editor-in-Chief

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