

Special Issue

Molecular Dynamics: Application of Computer Simulations in Soft Matter, Nano-Engineering and Biophysics

Message from the Guest Editor

This Special Issue seeks to provide insights into modern problems in soft matter, nano-engineering, and biophysics, with the help of molecular dynamics simulations. It aims to identify contributions that emphasize the importance of computer simulations for revealing the fundamental phenomena behind the processes in nature, as well as the application of MD simulations to practical engineering questions. Contributions from any area of soft matter, nano-engineering, and biophysics, are welcomed, including (but not limited to):

- Complex fluids, colloids, ionic liquids;
- Glasses, polymers, gels, surfactants;
- Porous, disordered, and functional materials;
- Biological membranes and biomolecules;
- Self-assembling structures, active matter, drug delivery.

We invite original research that addresses computational challenges in systems with non-equilibrium conditions, large fluctuations, strong coupling, non-local effects, active and non-potential interactions, coarse-graining needs, long relaxations, and phase transitions.

Guest Editor

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Deadline for manuscript submissions

closed (20 July 2022)



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Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

Editor-in-Chief

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