

Special Issue

Understanding the Nanoparticle-Biomolecule Interactions: Insight Form Computational Modelling and Atomistic Simulations

Message from the Guest Editor

Nanoparticles are enjoying rapid growth as promising tools for biomedical applications. In order to fully exploit their potential and reduce the gap between bench discoveries and clinical applications, precise control of the biological activity and the fate of nanoparticles is necessary. Computational simulation provides fundamental knowledge enabling us to unravel the underlying principles and elucidate the molecular mechanisms of specific interactions and of the dynamics that nanoparticles induce on biological molecules upon binding.

This Special Issue will cover some of the recent significant advances in the field of modelling and computational simulations of the interactions between nanoparticles and biomolecules. Reviews, full papers and short communications in this field are all welcome.

Keywords

- Nanoparticle biomolecule interactions
- Nanoparticle DNA interactions
- Nanoparticle membrane interactions
- Structure-function relationships
- Advanced molecular modelling techniques
- Molecular dynamics simulations
- Chemoinformatics

Guest Editor

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