Special Issue

The Application of Machine Learning to Molecular Dynamics Simulations

Message from the Guest Editor

Molecular dynamics allows for detailed study of the atomistic behavior of biomolecules, such as protein–ligand and protein–protein interactions and has played an important role in the field of drug discovery and development. Machine learning, through models like deep learning, accelerates the process, enabling faster predictions of key properties such as binding affinity, toxicity, and mechanisms of action. By combining machine learning algorithms with molecular dynamics simulations, we can achieve faster and more accurate simulations, leading to a deeper understanding of the properties and behavior of molecular systems. This Special Issue focuses on recent advances in machine learning to improve force fields, sampling, and property prediction in molecular dynamics simulations. The application of this approach can be primarily targeted at drug discovery, but can be extended to other aspects of protein structure and dynamics related to drug discovery. Innovative methods are also welcome to enhance the drug discovery process, the evaluation of mechanisms of action, and the study of atomistic details in biomolecular interactions.

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