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Molecular Dynamics Simulation of Biomolecular Systems

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Abstract: The group for computer-aided chemistry at the ETH Zürich focuses its research on the development of methodology to simulate the behavior of biomolecular systems and the use of simulation techniques to analyze and understand biomolecular processes at the atomic level. Here, the current research directions are briefly reviewed and illustrated with a few examples.

Keywords: Biomolecular simulation · Membranes · Methodology · Molecular dynamics · Proteins