Molecular Dynamics Simulations of Membrane Related Processes. Edition No. 1

Description: Molecular dynamics (MD) simulations of classical fluids have led to a revolution in our understanding of the equilibrium and non-equilibrium properties of fluids. In this book we have used MD method on fluids confined by membranes to study an equilibrium thermodynamic problem (solubility of gases in liquids) and a dynamic problem (permeation of gas in biomembranes). A simulation system with a selective permeable membrane in it to mimic a real experiment was developed. Computational studies were focused on gas solubility in equilibrated organic liquid systems and on the dynamics of gas permeation process through model biological membranes. When investigating gas solubilities, the MD method, intermolecular NMR (Nuclear Magnetic Resonance) chemical shifts were used to fine tune intermolecular potentials. In our studies on gas permeation, atomic simulations were coarse-grained to understand the basic gas permeation functions of a biomembrane. By reducing the degrees of freedom and employing suitable potentials, direct insight into collective phenomena in biological membranes at longer time and length scales were provided.


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