



Molecular Dynamics Services Section Home

History

The origins of molecular dynamics can be traced back to the early 20th century when researchers began exploring the behavior of atoms through mathematical equations. The advent of computers in the mid-20th century revolutionized the field, enabling simulations that were previously impossible. In the 1950s and 60s, computational pioneers like Metropolis and Alder laid the groundwork for simulating particle behavior. The development of molecular dynamics algorithms in the 1970s paved the way for simulating complex molecules and systems.

Alder and Wainwright

Their work on the "molecular dynamics" method marked the birth of computational simulations.
2.

Andreas Heuer

A pioneer in coarse-grained molecular dynamics, his work paved the way for simulating larger molecular systems.

Industrial Applications

1.

Protein Folding

It investigates protein folding pathways, providing insights into protein misfolding diseases.
3.

Drug Binding Kinetics

It predicts drug-receptor binding rates and off-rate constants.
5.

Membrane Proteins

It studies membrane protein dynamics, crucial for drug delivery and signaling.
7.

Catalysis Mechanisms

It unravels reaction mechanisms on catalytic surfaces.

9.

Protein Dynamics

It investigates conformational changes in proteins, crucial for function.

11.

Protein-Protein Interactions

It studies the assembly and dynamics of protein complexes.

13.

DNA Dynamics

It simulates DNA conformational changes and interactions with proteins.

15.

Surface Reactions

It models surface-catalyzed chemical reactions.

17.

Solvation Effects

It predicts solvation properties and solvent-induced effects.

19.

Quantum Dynamics

Molecular dynamics integrates quantum mechanical effects into classical simulations.