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Editorial

Modelling of Molecules

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Molecular modelling encompasses all methods, theoretical and computational, wont to model or mimic the behaviour of molecules. The methods are utilized in the fields of computational chemistry, drug design, computational biology and materials science to review molecular systems ranging from small chemical systems to large biological molecules and material assemblies. The molecular modeling is one of the applications which requires a well programmed computer system that would be working on the principal of atomistic level of the molecular structure as to perform ones molecular modeling. It can be achieved by considering the atoms as the smallest individual unit as accepting the molecular approach or by explicitly modelling protons and neutrons with its quarks, anti-quarks and gluons and electrons with its photons (a quantum chemistry approach).

Molecular mechanics is the comprisation of the Newtonian mechnaics along the exploration of the physical basis involved in the molecular model. Molecular modeling tends to describe the atoms (nucleus and electrons collectively) as the unit charge along with the associated mass. The collectivity of the molecules is described by the interaction among the atoms which are the vander waals force which is described by the Lennard-Jones potential. Coulomb's Law are responsible for the decvription of the electrostatics forces between the atoms. The locus of an atom is decided in the Cartesian Space and the velocity should be decided by the dynamical simulations. The atomic velocities are related to the temperature of the system, a macroscopic quantity.

The common force fields in use today are developed by using chemical theory, experimental reference data, and high level quantum calculations. Lower energy states are more stable and are commonly investigated due to their role in chemical and biological processes. It involves solving Newton's laws of motion, principally the second law, F =ma. The force on an atom is defined because the negative gradient of the P.E. function. The energy minimization method is beneficial to get a static picture for comparing between states of comparable systems, while molecular dynamics provides information about the dynamic processes with the intrinsic inclusion of temperature effects.

Molecules are often modelled either in vacuum, or within the presence of a solvent like water. Simulations of systems in vacuum are mentioned as gas-phase simulations, while people who include the presence of solvent molecules are mentioned as explicit solvent simulations. In another sort of simulation, the effect of solvent is estimated using an empirical mathematical expression; these are termed implicit solvation simulations.

Most force fields are distance-dependent, making the foremost convenient expression for these Cartesian coordinates. Yet the comparatively rigid nature of bonds which occur between specific atoms, and in essence, defines what's meant by the designation molecule, make an indoor frame of reference the most logical representation. Thus, it's quite common for computational optimizing programs to flip back and forth between representations during their iterations. While all conversion algorithms produce mathematically identical results, they differ in speed and numerical accuracy. Currently, the fastest and most accurate torsion to Cartesian conversion is that the Natural Extension Reference Frame (NERF) method.

Molecular modelling methods are now used routinely to investigate the structure, dynamics, surface properties, and thermodynamics of inorganic, biological, and polymeric systems. The types of biological activity that have been investigated using molecular modelling include protein folding, enzyme catalysis, protein stability, conformational changes associated with biomolecular function, and molecular recognition of proteins, DNA, and membrane complexes.

CONFLICT OF INTEREST

We have no conflict of interests to disclose and the manuscript has been read and approved by all named authors.

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