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Research Papers

MOLECULAR DYNAMICS: AN EFFECTIVE COMPUTATIONAL TOOL

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Abstract

A brief review about computer simulations has been presented in this article. The introduction of computers and its subsequent applications has changed the way of chemical calculations. The final section of article which highlights the future prospects of computational techniques will certainly motivate the researchers to purse research in theoretical chemistry.

Keywords: Computational techniques, Molecular dynamics, Monte Carlo method, equilibrium and non-equilibrium properties.

1. INTRODUCTION

Since the mid of 20th century, there has been tremendous growth in the computational techniques. The rapid increase in the computational power has helped in the development of theory which supported the experimental findings and , in some cases predicted the properties at molecular level for which experimental determination is very costly and time consuming, sometimes, even impossible.

Computational methods are used in chemistry are basically used to calculate two types of properties, namely, equilibrium and non-equilibrium properties. Examples of former are free energy, temperature, density, average structureetc.,whereas, shear viscosity, transport coefficient etc are determined as non-equilibrium properties. For all the properties, the accuracy level obtained depends on the simulation techniques and the parameters which have been used in those techniquesto model the actual system under study.

Computational techniques have proved to be immensely helpful in chemistry for solving Schrodinger's equation at various levels of approximations. The information obtained at atomic and molecular levels supplemented the understanding of experimental findings. With the use of sufficiently accurate parameters (tomodel the system under study), various properties of the system can be derived using statistical mechanics [1-5].

2. MOLECULAR DYNAMICS AS AN EFFECTIVE COMPUTATIONAL TOOL

Molecular dynamics, along with Monte Carlo and energy minimization calculations is an effective tool the study of condensed phases such as liquids, liquid crystals, polymers etc.

The first molecular dynamics simulations were performed by Alder and Wainwright [6] of the hard-sphere. The properties of the systems such as the pressure and the radial distribution functions were computed and analyzed. In 1964, Rahman [7] performed MD simulations of liquid Argon to calculate

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equilibrium properties and diffusion coefficient using particle correlation function.

With the advent of computational power, the technique of MD simulation was effectively applied for rigid polyatomic molecules and flexible molecules under certain sets of conditions and constraints [8-9]. Subsequently, the technique became applicable to biological systems involving nucleic acid and proteins. The accuracy of results obtained by these studies were essentially determinedby the models (force fields) and the duration of simulations.

For a complex molecular modelling, there are two basic problems:

i) The first problems, is the search for configuration space with global low (free) energy region which is populated by the system in equilibrium. The success of a molecular modelling technique depends on its ability to search and describe that part of configuration space which is accessible to the system at the given temperature.

ii) The second problem is the derivation of a sufficiently accurate interaction energy function for the system under study.

The complex chemical/ biochemical systems can be considered to be made up of two parts; a nuclear part containing nuclei with negligible size and an electronic part containing electrons moving around (Born- Oppenheimer approximation). In other words a complex molecular system can be described as a system of atoms moving in a potential field due to many body atom-atom interactions. Within the system, the intra-molecular interactions include bonded and non-bonded interactions. The bonded interactions consist of covalent bond stretching, bond angle bending and torsional angle interactions. The non-bonded interactions are generally limited to two-body terms.

The original molecular dynamics simulations were carried out using micro canonical ensemble (constant NVE) and then later extended to other ensembles such as canonical [10]and isothermal-isoenthalpic ensemble [11] using the generalized Lagrangian method. The technique was later developed to calculate statistical properties such as the entropy, chemical potential etc., followed by application of MD techniques to study non equilibrium properties for example, calculation of transport properties using the time correlation function based on Green –Kubo relationship.

The Molecular Dynamics is a versatile computational techniques. It can be used for validation purpose by adjusting the force field parameters to reproduce condensed phase data. It can also be used to predict properties which are otherwise, difficult to obtain by experimental work, using suitable modelling of the system. The method can be used to check the accuracy of statistical mechanics theories as well. MD simulation is extremely valuable tool to study diffusional behavior and to obtained structural information at molecular level.

3. THE FUTURE PROSPECTS

The accuracy of results obtained by molecular dynamics simulations are essentially depends on the models (force fields) and the duration of simulations.

Advances in more accurate use of force field is an important need in future. Attempts have been made in the recent works and more are expected, which would account for the effect of changes in bond lengths and bond angle on torsional potentials. Also, efforts are needed for the better handling of electrostatic potential around a molecule. Simulation where polarization effects have been taken into consideration are needed on a larger scale in future as well.

The exponential rise in the computational power/ facilities have made possible to carry out simulation studies for a considerable long duration of time, thereby increasing the accuracy of findings. Additionally, long duration simulations with larger time steps are essential to study the complex biological systems.

In order to enhance the reliability and applicability of computational results, measures have been taken to include quantum mechanics with molecular dynamics which accounts for the effect of nuclei in electronic structure calculations, such as Carl-Parrinello simulations. There is need of more such studies to predict, validate and test various properties.

The technique of MD simulations can also be applied to complex condensed systems where small portion of systems can be treated quantum mechanically and rest of the systems are simulated using classical molecular dynamics. Such hybrid methods are expected to provide a much better

predictions of properties and can play vital role in validation and testing of statistical mechanics theories.

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