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Molecular Modeling

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Abstract
In this paper, the modelling of molecule is presented. Chemistry, as the central science, utilizes models in virtually every aspect of the discipline. Integral to the progress of chemistry has been its ability to draw from physics, mathematics, statistics, and computer science to develop new sub disciplines, such as computational chemistry. As computing hardware has become faster and more accessible, so to have techniques to perform modelling and simulations of molecular systems. Software systems today assist researchers in the study of molecular systems and provide mechanisms for deriving a rigorous and consistent explanation for the chemical or biological behaviour observed or help the researcher to develop a model for predictions. Molecular modelling is a field that encompasses a wide range of theoretical and computational methods used to represent the structure and behavior of molecules, ions, and particles. These models can be classified based on their length and time scales, ranging from electronic-level models to continuous-level models. One of the main applications of molecular modelling is in drug discovery, where it can be used to predict the activity and behavior of molecules in the body, aiding in the design of new drugs. Additionally, molecular modelling plays a crucial role in materials science, where it can be used to design new materials with specific properties, such as strength, flexibility, and conductivity. With advances in computing hardware and software, molecular modelling has become an increasingly powerful tool in the fields of chemistry, physics, biology, and materials science, allowing researchers to gain a deeper understanding of the behavior of molecules and particles at the molecular level. The work done & presented in this paper is the result of the mini-project work that has been done by the first sem engineering students of the college and as such there is little novelty in it and the references are being taken from various sources from the internet, the paper is being written by the students to test their writing skills in the starting of their engineering career and also to test the presentation skills during their mini-project presentation. The work done & presented in this paper is the report of the assignment / alternate assessment tool as a part and parcel of the academic assignment of the first year subject on nanotechnology & IoT.
Keywords: Nano, Molecule, Model, Biology, Physics, Chemistry, Behavior

Introductory notes

Science is essentially the process of creating models that explain and predict observations, and chemistry relies heavily on models in its various applications. Molecular modeling is a prime example of the use of models in chemistry. Molecular modeling, which includes computer-assisted molecular modeling (CAMM), has evolved as a result of convergence of various techniques from different fields [1]. Modern computational tools allow researchers to study a broad spectrum of molecular systems and make property predictions with consistency and accuracy. The increasing ease of use of molecular modeling software, coupled with the rise in computing power and the incorporation of these tools

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into curricula, has resulted in a surge of research in this area [2]. However, it is crucial for users to have a good understanding of the origins and strategies of molecular modeling and not simply rely on "black box" computations. This chapter provides a guide to the literature of molecular modeling to help researchers use these powerful tools effectively [3].

Primary Objective

The primary objective of molecular modeling is to establish a clear relationship between the molecular formula, the 3D topology or geometric constitution, and the observed or predicted properties of a chemical compound. Molecular modeling involves the use of computer graphics software and hardware to facilitate the representation and manipulation of 3D arrays of atoms. To carry out a molecular modeling study, several steps must be followed [4]. First, the problem is formulated, and initial estimates of the hardware and software resources needed are developed. Second, the structure-generation methods are defined, including on-the-fly 1D or 2D to 3D conversion, retrieval from local or online databases, and checking for sterochemistry, tautomerism, and ionization state. Third, structures are evaluated to determine if they require cleanup or full energy minimization, and are sent to a structure optimizer as required. Fourth, structures are sent to an initial empirical molecular descriptors generator, and the distribution of computed properties is evaluated to decide if multiple conformations are needed [5]. Fifth, if quantum-based descriptors are required, structures are routed through appropriate software systems to generate them, and statistical distributions are evaluated and reiterative analysis is carried out as required. Finally, descriptors are used to sort and prioritize structures for evaluation by next level protocols such as reactivity analysis, kinetic properties, ligand docking, structure-bioactivity/toxicity correlations, structure-property relationships, and spectroscopic simulation which is shown in Fig. 1 [6].

Use of computer graphics for molecular modelling

Computer graphics tools have had a profound impact on the ability of molecular modelers to compose a modeling study and address all aspects of the work, ranging from generating 3D structures from 2D sketches to statistical quality control of computed properties via visualization of multidimensional data. The availability of computing software and hardware systems has continued to increase, with even a simple device like an iPad capable of handling the display of macromolecular systems. Figures 2-6 in the article provide increasingly complex and useful structural representations that illustrate the enhancement in the visualization of structure and properties, such as a ball and stick drawing of the drug ZantacTM (ranitidine) and a CPK shaded solid surface for ranitidine [7].

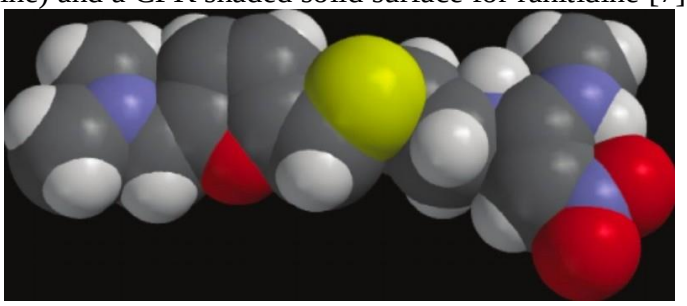

Fig. 1: A CPK rendering of the ZantacTM (ranitidine) molecule. Color coding Rendered using Spartan’14 v 1.1.4 (Mac).

Development of model of a molecule

Molecular modelling encompasses all methods, theoretical and computational, used to model or mimic the behaviour of molecules [1] The methods are used in the fields of computational chemistry, drug design, computational biology and materials science to study molecular systems ranging from small chemical systems to large biological molecules and material assemblies. The simplest calculations can be performed by hand, but inevitably computers are required to perform molecular modelling of any reasonably sized system. The common feature of molecular modelling methods is

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the atomistic level description of the molecular systems. This may include treating atoms as the smallest individual unit (a molecular mechanics approach), or explicitly modelling protons and neutrons with its quarks, anti-quarks and gluons and electrons with its photons (a quantum chemistry approach) which is shown in the Fig. 2 [8].

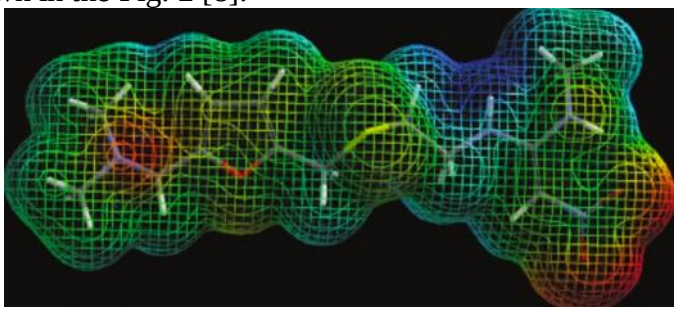

Fig. 2 : Mesh surface rendering of the ZantacTM (ranitidine) molecule, using the same element color scheme. The Electrostatic Potential computed at the 6- 31G HF-SCF basis set level is mapped onto the mesh surface. The color ranges from most negative (red) to most positive (purple/blue) following the ROYGBIV protocol. Rendered using Spartan'14 v. 1.1.4 (Mac).

Molecular mechanics

Molecular mechanics is one aspect of molecular modelling, as it involves the use of classical mechanics (Newtonian mechanics) to describe the physical basis behind the models. Molecular models typically describe atoms (nucleus and electrons collectively) as point charges with an associated mass. The interactions between neighbouring atoms are described by spring-like interactions (representing chemical bonds) and Van der Waals forces. The Lennard-Jones potential is commonly used to describe the latter. The electrostatic interactions are computed based on Coulomb's law. Atoms are assigned coordinates in Cartesian space or in internal coordinates, and can also be assigned velocities in dynamical simulations [9]. The atomic velocities are related to the temperature of the system, a macroscopic quantity. The collective mathematical expression is termed a potential function and is related to the system internal energy (U), a thermodynamic quantity equal to the sum of potential and kinetic energies. Methods which minimize the potential energy are termed energy minimization methods (e.g., steepest descent and conjugate gradient), while methods that model the behaviour of the system with propagation of time are termed molecular dynamics [10].

Simulated results

Simulation is carried out in the Spartran environment, the coding is done, the program is run & the simulation results are observed as shown in the Fig. 3.

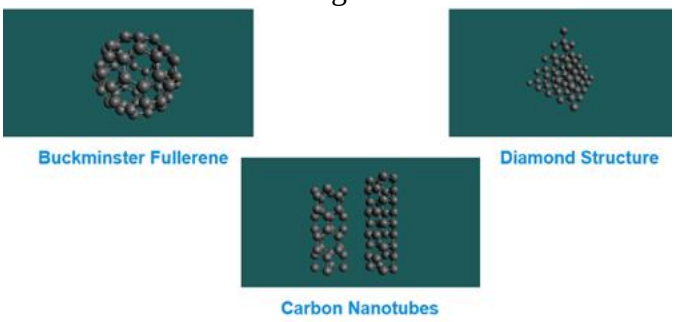

Fig. 3 : Simulated results using the software tools

Conclusions

In conclusion, molecular modelling is a powerful tool that allows scientists to study the behavior and properties of molecules and their interactions with other molecules. It has evolved significantly since the mid-1960s with the development of graphics software and hardware and the growth of computing resources. Molecular modelling provides researchers with the ability to generate and evaluate 3D arrays of atoms, analyze molecular properties, and predict new ones. The use of molecular modelling

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has expanded rapidly and has become more accessible to researchers due to advancements in computing technology and the introduction of modelling tools in undergraduate and graduate curricula. However, it is essential for researchers to have a good understanding of the origins of the methods and strategies of molecular modelling to ensure that these techniques are used effectively. The continued development of molecular modelling will undoubtedly lead to new discoveries in many fields, from drug design to material science, providing insight into the fundamental behavior of molecules and their interactions with the world around us.

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