



P-ISSN2349-8528  
 E-ISSN 2321-4902  
 IJCS 2016; 4(2): 46-47  
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 Received: 15-01-2016  
 Accepted: 16-02-2016

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## Quantum chemistry is a path way to develop Nano medicine

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### Abstract

Interacting with biological molecules at nano scale broadens the field of research and application. Interactions of nanodevices with bio molecules can be understood both in the extracellular medium and inside the human cells. Quantum mechanical models describe the electrons statistical positions. Thus quantum chemical calculations can be used to predict chemical reactions.

**Keywords:** Quantum chemical calculation, Nano particle, Nan medicines

### 1. Introduction

Near future scientist can show that chemical bonding in the magnetic fields of small, compact stars is different from that of earth. Their calculations pointed to a completely new bonding mechanism between two hydrogen atoms. Researcher's showed <sup>[1]</sup> earlier what happens when atoms and molecules are exposed to extreme conditions by the help of quantum chemical calculations <sup>[2]</sup>. Professor Trygve Helgaker, design of a computer system for calculating quantum chemical reactions in molecules. Quantum chemical calculations are required to see the behaviour of electrons trajectories within a molecule. When UV radiation applies in to the cell it increases the energy level hence some molecules splits. This extra energy will affect the behaviour of electrons and can destroy the chemical bonding within the molecule. The quantum chemical models are used to produce a picture of the forces and tensions at play between atoms and the electrons of a molecule <sup>[3]</sup>. Electrons are not only particles, but wave as well, which can be many places at a time. It is difficult to track them. Quantum mechanical models describe the electrons statistical positions which sketch the probable location of each electron can be located. Thus quantum chemical calculations are often more accurate than what is achievable experimentally quantum chemical calculations can be used to predict chemical reactions.

Methods: - There are two important areas within computational chemistry are molecular mechanics and electronic structure theory. (a) Computing the energy of a particular molecular structure. (b) Performing the geometry optimizations which locate the lowest energy molecular structure in close proximity. Computing the vibrational frequencies of molecules resulting from interatomic motion with in the molecule. Gaussian-03 is a computational chemistry software program used for performing the quantum chemical calculations.

Molecular electrostatic potential: - MEP is a plot of electrostatic potential mapped on the iso-electron density surface, simultaneously displays molecular shape, size and electrostatic potential values for the molecules. It is used in studies of biological recognition and hydrogen bonding interactions. Type equation here.

$$n(r) = N \int d^3r_2 \int d^3r_3 \dots \int d^3r_N \psi^*(r_1, r_2, \dots, r_N) \psi(r_1, r_2, \dots, r_N)$$

Now quantum chemical calculations can be made what happened within the molecule of up to 400 atoms. Hence researchers getting close to a level which enables them to study the quantum mechanics of living cells.

Molecular electrostatic potential (MEP):- MEP is a plot of electrostatic potential mapped on the iso-electron density surface, simultaneously displays molecular shape, size and electrostatic potential values for the molecules. It is used primarily for predicting sites and relative reactivities towards electrophilic attack and in studies of biological recognition and hydrogen bonding interactions.

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**1.1 Hunting for the electrons in bio molecules:** According to literature review an insulin molecule consists of 782 atoms and 3500 electrons. All electrons repel each other, while at the same time being pulled towards the atomic nuclei. The nuclei also repel each other but molecule remains stable. To study the

molecule to a high level of precision, we consider how all of electrons move relative to one another. Such calculations are referred to as correlated and are very reliable. Development of nanotechnology in medicine.

Year	Development of nano particles in medicine
2002	Feynman awarded for using DNA to enable the self-assembly of new structures for advancing our ability.
2004	Nanotechnology was awarded for designing stable protein structure
2005-10	3D nano system, 3D networking and active nano products that change their state during use were prepared
2011	Era of molecular nano technology study
2015-	Quantum chemical calculation may be used to produce tomorrow's drugs.

**1.2 Importance in Nano medicines:** Quantum chemical calculation provides support for interpreting and planning experiments. Enzymes are molecular catalysts that boost the chemical reactions within our cells. In nanomedicine we need to understand physical phenomenon on a nano scale forming as correct a picture as possible of molecular phenomena. Quantum chemical calculations will teach us more about how proteins go about their tasks, step by step the calculations look at activation energy. It is important to understand the chemical reaction patterns in biological molecules in order to develop new drug. Interacting with biological molecules at nano scale broadens the field of research and application. Interactions of nanodevices with bio molecules can be understood both in the extracellular medium and inside the human cells. Nano materials like nano particles and dendrimers are called as nano biopharmaceuticals are used for targeted controlled delivery. Nanoparticles such as quantum dots, with quantum confinement properties, such as size-tunable light emission can be used in conjunction with magnetic resonance imaging, to produce exceptional image of tumour sites. In neuro degenerative disorders the delivery of CNS therapeutics, various nano carriers such as, dendrimers, nano gels, nano emulsions, liposome's, polymeric nanoparticles, solid lipid nanoparticles and nano suspensions have been studied.

nonmaterial with endogenous the therapeutic and diagnostic functions. *Cancer Nano.* 2010; 1:13-18.

**2. Conclusions:** The properties of nano materials can greatly influence their interactions with bio molecules and cells, due to their peculiar size, shape, chemical composition, surface structure, charge, solubility and agglomeration. Nano particles have unique physicochemical and biological properties. Proper use of the knowledge on that structure and the ability by the help of quantum chemical calculation put them to practical use in treatment, diagnostics and disease prevention will benefit the health quality and quality of life of the patients.

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