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COMPUTATION MODELLING METHOD OF NANO MOLECULE

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Abstract -- This study demonstrates the computation of structures and properties of a nano molecule using density functional theory. Computational methods dealing with the prediction and analysis of spectroscopic measurements and of their interpretation in terms of stereo-electronic, environmental, and dynamical effects. The basis of nano cluster model and quantum chemical methods of different level is critically discussed. This work illustrated by a great deal of theoretical *ab initio* and semi-empirical calculations and basis-set choices.

Keywords: Ab-initio, DFT method, Guassian, Basis set.

I. INTRODUCTION

The future applications of nanotechnology in high-tech industries require deep understanding of the theoretical and computational aspects of all kinds of materials and devices at a nanometer scale.[1] Computational chemistry uses the results of theoretical chemistry, incorporated into efficient computer programs, to calculate the structure and properties of nano molecules and solids. Theoretical nanophysics group studies the quantum and classical phenomena in small electronic systems, with a focus on orbitals.[2]

The approach of nano scale modeling using simulation methods of MATLAB. Ab initio computer programs such as ATMOL, GAUSSIAN, IBMOL, POLYAYTOM and Cache are being used to speed up calculations of molecular orbitals. The commercial package GAUSSIAN is considered by most to be the "industry standard", although other packages like Spartan, Hyper hem are challenging Gaussian for computational performance. Gaussian is the benchmark by which all other ab initio codes are measured. The primary advantage of ab initio methods is the accuracy with which calculations are performed. To the degree that a researcher needs to know a property that most accurately matches experimental data or that most approximates a theoretical prediction, the ab initio method is chosen.

II. AB-INITIO CALCULATIONS

Ab-initio (Lain - "from first principles") involves mathematical modeling, based on Schrodinger's equation. Using several constants such as speed of light, Planck's constant and mass of the electrons and nuclei, one can use *ab initio* methods to calculate a wide variety of properties like the energy of nano molecule, its vibratioal frequencies, and thermodynamic properties [13]. Ab-initio is regarded as the most accurate and precise of all of the currently available methods in molecular modeling. These methods are currently applied largely to small molecular systems [14].

2.1. HARTREE-FOCK THEORY

A rationale on how nano particles of different sizes, shape, structure and chemical properties can affect the organization and functions of nano-machinery of cells is also presented. Virtually all ab-initio calculations start out at the Hartree-Fock, named after those physicists who developed the system. A set of approximate orbitals (a basis set) is chosen for all the electrons in the system [15]. The Schrodinger equation for the selected electron is calculated, resulting in a new, more accurate orbital for that electron. The procedure is repeated for all the other electrons in the system. Finally, the calculations are considered "completed", since the orbitals are now considered being "self-consistent". [16]

2.2. DENSITY FUNCTIONAL THEORY

The DFT was set forth in the work of Hohenberg and Kohn [17]. Zeigler report that the use of DFT in the ab initio calculation of small molecular properties has recently increased dramatically [18]. It can be attributed to the development of new and more accurate density functional aid with increasing efficiency by DFT computations relative to other *ab initio* methodologies [19]. Chacon Villalba et al reported quantum chemistry irrational study using density functional theory (DFT). A number of Density functional methods like B3LYP, B3P86, B3PW91, BH and H, BH and HLYP are available. The density functional method used in this study is B3LYP. [20]

2.3 B3LYP

The B3LYP respondents the hybrid Becke -3-Lee-Yang Parr co relational function. This functional is a hybrid of exact (HF) exchange with local and gradient corrected exchange and correlation terms, as first suggested by Becke. The exchange - correlation functiona proposed and tested by Becke [21]

$$_{Exe} = (1\text{-}a_0)\ E_x^{LSPA} + a_0 E_x^{HF} + \Delta E_x^{B88} + E_c^{LSDA}\, a_c \Delta E_c^{PW91}$$

Here ΔEx^{B88} is Becke's gradient correction to the exchange functional coefficient and ΔE_c^{pw91} is Perdew - wang gradient correction to the correlation functiona. He suggested the coefficients as $a_0 = 0.2$. $a_x = 0.72$, $a_c = 0.81$ based on fitting to heats of formation of small molecules.

III. BASIS SET CHOICES

Slater-type orbital's (SFOs) were used in *ab initio* calculations in the early stages. But, for nano, the evaluation of the resulting one- and two- centered integrals presented a major computation .This can be effected by adding additional d functions or a combination of "d" and "p" functions. This ombination of two functions produce two new orbitals. One way of designating these polarized basis sets is by listing the functions added i.e. 6-31G (d,p), which adds "d" functions to the non-hydrogen atoms and "p" functions to the hydrogen atoms. This notation is also given as 6-311G. [22] The combination of triple Zeta function 6-311G (d, p) is used in the present investigation for calculating the vibrational assignment of the compounds chosen.

3.1. Geometry Optimization

Many systemic mathematical procedures exist to find a local minimum of a function of several variables. These procedures will find a local minimum in the neighborhood of the initially assumed geometry. [23] The process of finding such a minimum is called geometry optimization in energy minimization. For a molecule with several conformations, one must repeat the local minimum search procedure for each possible conformation, so as to locate the global minimum.

VI. CONCLUSION

Computational nanotechnology concludes by discussing future directions in the field, highlighting the importance of the algorithms, modeling software, and computational tools in the development of efficient nano scale systems. It is used to validate hypotheses that may not be accessible through traditional experimentation. This modeling method contributes the tracking of nano scale structures in cells, effects of various forces on cellular behavior.

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