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A Review of the Computing Study of Non-Covalent Interactions and its Applications

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ABSTRACT

Noncovalent interactions are crucial to biological processes. Noncovalent interactions help with anything from molecular recognition to molecular assembly to enzyme catalysis to the dynamic behaviour of biomolecules. Applications of noncovalent interactions in problems relating to many domains of chemistry, biology, and physics have become inevitably significant in recent years and are on the approach of becoming even more so. Noncovalent interactions that are dominated by electrostatic contributions have received the most attention and coverage due to their ubiquity and binding strength. Electrostatic interactions are directed and have a considerable range. However, due to the fundamental long range impactful character of electrostatic contributions, the directional elements of electrostatic dominated noncovalent interactions have been completely disregarded in the literature thus far. This thesis focuses on the importance and directional nature of long-range electrostatic interactions in order to completely understand the electrostatic contributions. We have given a brief overview of noncovalent bonds and their role in chemistry in this chapter. We also went over a brief history of the scientific literature to show how awareness of the importance of long-range electrostatic interactions has evolved over time.

KEYWORDS: *Computing, Non-Covalent, Interactions, Applications, Biological Processes, Molecular Recognition.*

INTRODUCTION

The weak forces of attraction that are created between two distinct things or among the many pieces of the same entity are referred to as non-covalent interactions. Despite the fact that noncovalent interactions are far less powerful than covalent bonds, the latter play an essential part in the study of material science, chemistry, and biology. These interactions are present in bio-molecular systems such as proteins and nucleic acids, as well as supramolecular systems such as polymers, in which the sets of molecules are linked orderly through various types of non-covalent interactions. (Nziko, 2013:16) Even though the experimental methods have been used to study of the non-covalent interactions, the detail and origin of the non-covalent interactions can now be studied using theoretical and computational methods. Even though the experimental methods have been used to study of the non-covalent interactions. The increase in computer capacity has resulted in the creation of trustworthy computational tools, which are now utilised in the process of characterising an interaction that is non-covalent.

The computational methods are not only used to calculate the energetic of molecules, but they are also used to calculate the energy decomposition in various types of fragments of energies, cooperativity, electrostatic potential, Atoms in Molecules (AIM), Natural Bond orbital (NBO), and electron density redistribution. In other words, the computational methods are used to do more than just calculate the energetic of molecules. When it comes to the investigation of non-covalent interactions, one can consider the interaction energy to be the single most crucial piece of information. When two monomers, A and B, are allowed to interact with one another, the interaction energy that is generated as a result of their aggregation can be calculated as the difference between the energy of the AB complex and the sum of the energies of monomer A and monomer B. This difference is referred to as the interaction energy delta. Because of orbital overlap in the AB complex, the resultant interaction energy is typically calculated to be higher than it actually is. The counter poise process is typically used to correct this overestimation that has been made. People frequently believe that electrostatic, charge transfer (induction), and/or dispersion energy are the sources of the interaction energy. (Otero-de- la, 2012). Non-covalent interactions come in a variety of forms, including hydrogen bonds, van der Waals interactions, hydrophobic interactions, ion-induced dipoles, and dipole-induced dipoles. Each form of non-covalent interaction has its own unique geometry, strength, and specificity characteristics. In a table that classifies interactions based on their levels of energy, the van der Waal interaction will be located

toward the bottom of the table. The term "van der Waal interaction" is frequently and occasionally used in a very general sense to refer to the entirety of "intermolecular contact." The London forces are a subtype of van der Waals interactions that are caused by the dynamic interactions between transient multipoles in molecules that do not include permanent dipoles. These interactions give rise to the London forces. The degree to which molecules can be polarised influences how strong the London-van der Waal interaction is. [Case in point:] [Case in point:] It was discovered that the only thing responsible for keeping He atoms attached to one another was the London dispersion forces. (Aziz, 1991:94).

1. Noncovalent interaction types and examples-

Electrostatic, dispersion (London dispersion), polarization (induction), exchange repulsion (Fermi repulsion), and donor acceptor charge transfer interactions are some of the physically well characterized factors that go into noncovalent interactions (covalent contribution). None of these factors are physical observables, despite the fact that each of them has been extremely thoroughly specified. The scope of these contributors' influence may be broad or narrow, depending on the underlying characteristics that they bring to the table. Due to the fact that the overlap of molecular orbitals (or the transfer of charge from one partner to another) is where short range interactions get their start, it follows that these interactions do not act over great distances. In molecular dynamics simulations, the forces that are regarded to be short range are those that have a reduction in strength with increasing distance that is faster than r- d (where d represents the dimensionality of the system, which is typically 3).

2. Interplay of cooperativity in noncovalent processes-

It has been shown that the strength of a noncovalent interaction is greatly dependent on the local arrangement of atoms in bonded partners as well as the local chemical environment. This is something that can be seen. In addition, it has been discovered that the mutual contacts that occur between various units that are involved in noncovalent interactions are not additive. For instance, the average bond strength of hydrogen bonds in water clusters grows as the bond length simultaneously decreases, and this strength is increased by a factor of two in a decamer. It is believed that cooperativity, non-cooperativity, and anti cooperativity in noncovalent interactions are the causes of this nonadditivity in noncovalent interactions. It is claimed that two noncovalent interactions are cooperative toward one another if they help each other become stronger, whereas it is said that they are anticooperative toward one

another if they help each other become weaker. The concept of cooperation denotes the fact that the combined amount of energy.

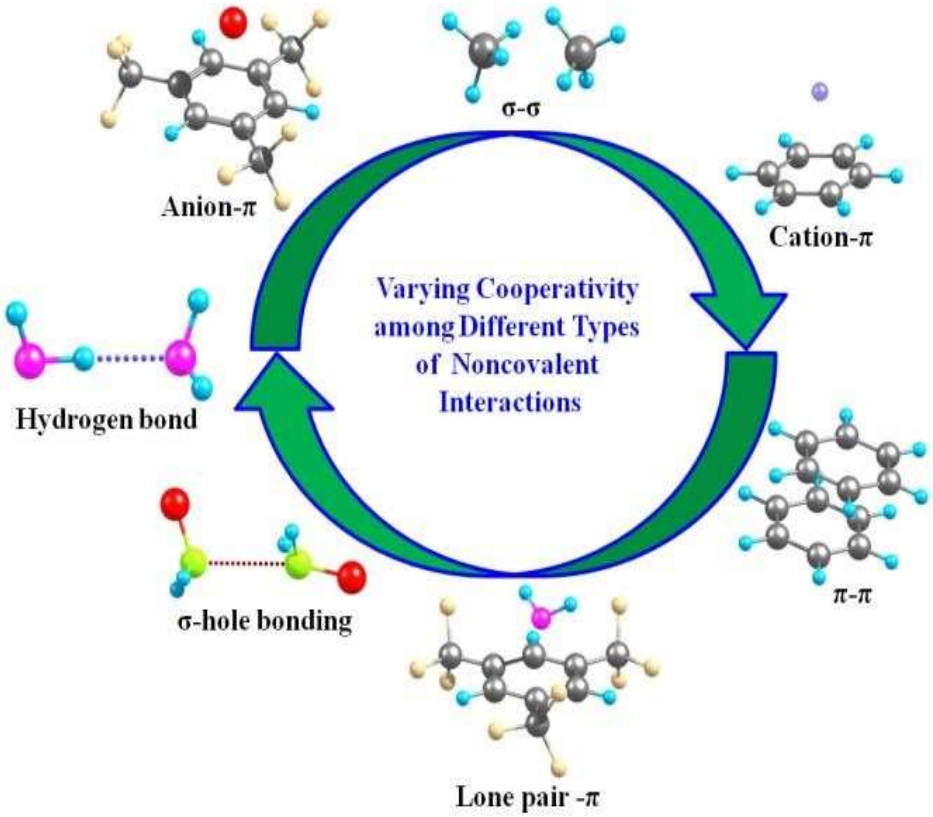

Figure 1: Representation of Several Noncovalent Interaction Types And A Common Cooperative Trend Among Them

3. Schematic representation of non-covalent interactions-

Three dots (...) rather than a whole line, which denotes a covalent link, depict noncovalent interactions. Covalent bonds between hydrogen and oxygen atoms in water molecules, for example, will be labelled as H-O, whereas a hydrogen bond between two water molecules will be denoted as H...O.

4. Some general nomenclatures-

The development of any type of bond is related with the release of energy, which accounts for the system's stabilization by the quantity of bond energy or bond dissociation energy. Bond dissociation energy is commonly used to describe the strength or stability of covalent bonds. However, there is no universal scale for determining the strength of noncovalent bonding. In general, the strength of noncovalent bond/bonds is described in terms of the

association constant, which accounts for the degree of production of the noncovalent bonded complex from the corresponding separated partners in experimental approaches.

5. Quantum Chemical Methods for Non-covalent Interactions-

Understanding numerous aspects of molecular systems requires an efficient and precise description of noncovalent interactions. Noncovalent interactions, like covalent interactions, can be explored using traditional quantum chemistry methods. In studying noncovalent interactions, two fundamental quantum chemical techniques have been widely used: I the ab initio wave function approach and (ii) density functional theory (DFT). Other options include semi empirical molecular orbital (MO)-based approaches and classical methods (atomistic molecular dynamics, coarse grained force fields, and continuum mechanics). Classical methods are based on classical mechanics, which does not explicitly consider electrons, and are hence less advanced than quantum chemical methods. Unfortunately, the efficacy and precision of these procedures do not complement one another. Depending on the system size and available computational resources, one must pick and choose among these options. At a high level, electron correlation wave function theory, such as CCSD(T), accurately characterizes all energy contributors of noncovalent interactions28, and is hence regarded as one of the finest ways for dealing with noncovalent interactions. These approaches, however, are computationally exceedingly expensive and cannot be applied to even moderately sized molecular systems.

6. Electro static Dominated Non-covalent Interactions-

Some noncovalent interactions, as detailed in are dominated by electrostatic contributions. This suggests that the electrostatic term accounts for the majority of their binding energy. The classic hydrogen bond is the best example of this type. This category also includes non-classical hydrogen bonding of type X-H (extremely polar)... -hole bonds are another example. The electrostatic dominated noncovalent interactions between ion-pairs in solutions can also be explored. Long-range interactions dominated by electrostatics have been developed. It has also been demonstrated that electrostatic contributions in hydrogen bound systems have a long-term effect on binding. The parts that follow will go over various aspects of electrostatic dominating noncovalent interactions.

7. Hydrogen bonding-

The most common type of noncovalent contact is hydrogen bonding. Hydrogen bonds are commonly described as X-H...Y, where X is an atom with greater electronegativity than the H atom and Y is an electron-rich species: any Lewis base. In this case, Y is known as the hydrogen bond acceptor because it absorbs H in a hydrogen bond, while X-H is known as the hydrogen bond donor. It should be emphasised that the hydrogen bond does not just refer to the H...Y interactions. Instead, the entire X-H...Y assembly is referred to collectively as a hydrogen bond. Hydrogen bonds are classified into two types: classical hydrogen bonds (when Y is an electronegative atom with a single pair of electrons on it, such as the hydrogen bond between water molecules) and non-classical hydrogen bonds (when Y is a -electron rich moiety, such as in the case of the XH... interaction, where X = O, N, C, halogens). Classical hydrogen bonds are found all across nature and are thought to be predominantly electrostatic in nature. Figure 2 depicts a representative example of a classical hydrogen bond. Primary interactions are electrostatic interactions between hydrogen bond acceptors and donors that are directly involved in hydrogen bonding with each other. Secondary electrostatic interactions are defined as electrostatic interactions between any pair of atoms between two partners that are not directly involved in hydrogen bonding. Long range electrostatic interactions relate to all types of electrostatic interactions (including primary and secondary interactions).

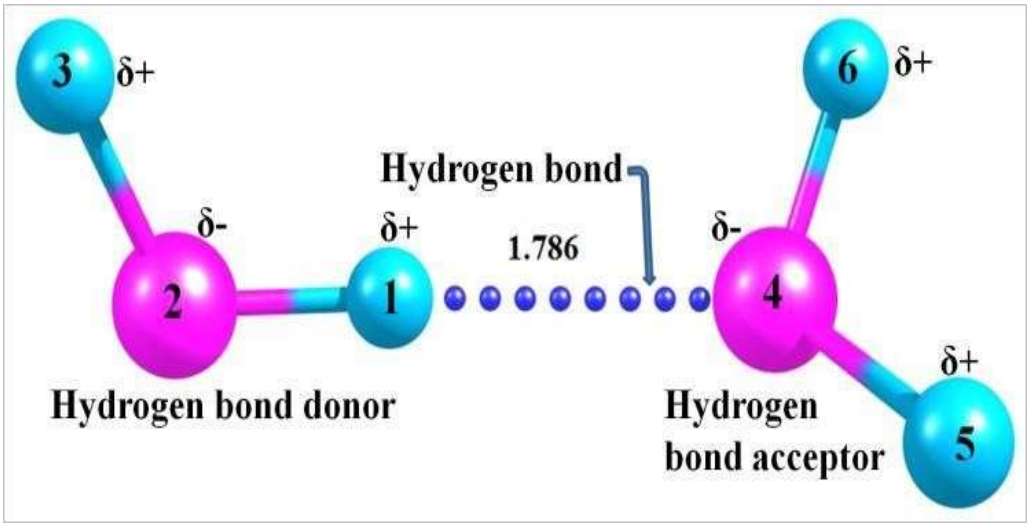

Figure 2: Turbomole 6.4 was used to optimise the geometry of the water dimer COSMO (water)/PBED3/TZVP level of theory

LITERATURE REVIEW

Boris B. Averkievetal.,(2010)- Studied that the structures of $Pd(PH_3)_2$ and $Pt(PH_3)_2$ Complexes with ethane and Conjugated C_nH_{n+2} systems (n=4,6,8, and 10) were studied.Their binding energies were calculated using both wave function theory (WFT) and density functional theory (DFT). Previously it was reported that the binding energy of the alkene to the transition metal does not depend strongly on the size of the conjugated C_nH_{n+2} ligand, but that DFT methods systematically underestimate the binding energy more and more significantly as the size of the conjugated system is increased. Its results show that recently developed density functional predict the binding energy for these systems much more accurately.

Maruti J Dhanavade et al., (2013) Cysteine protease is known to degrade amyloid beta peptide, which is a causative agent of Alzheimer's disease. This cleavage mechanism has not been studied in detail at the atomic level. Hence, a three-dimensional structure of cysteine protease from *Xanthomonas campestris* was constructed by homology modeling using Geno3D, SWISS-MODEL, and MODELLER 9v7. This model was then used further for docking and simulation studies. The molecular docking study revealed that Cys17, His87, and Gln88 residues of cysteine protease form an active site pocket similar to human cathepsin B. Then the docked complex was refined by molecular dynamic simulation to confirm its stable behavior over the entire simulation period.

The molecular docking and MD simulation studies showed that the sulfhydryl hydrogen atom of Cys17 of cysteine protease interacts with carboxylic oxygen of Lys16 of A βpeptide indicating the cleavage site. Thus, the cysteine protease model from *X. campestris* having similarity with human cathepsin B crystal structure may be used as an alternate approach to cleave Aβ peptide a causative agent of Alzheimer's disease.

Benam M R et. al., (2014) In this paper the effect of pressure on the structural and electronicproperties of cubic-$LaAlO_3$ including the equilibrium lattice constant, bulk modulus, derivative of bulkmodulus and band structure have been calculated by density functional theory (DFT) using GGA, LDA, and PBEsol exchange correlation potentials. It is found that the change of the lattice constant with pressure has an exponential behavior: with increasing pressure, the lattice constant Decreases first sharply at low pressures, and then

more slowly at high pressures. Furthermore, the lattice constant calculated by the PBEsol method and the bulk modulus calculated by LDA and PBEsol methods are closer to the available experimental values than those obtained using other exchange correlation potentials. Regarding the electronic properties, it is shown that an increase in pressure increases the band gap, the change being 0.26 eV at 34.00 GPa. The total density of state (t-DOS) calculations demonstrate that increasing pressure has a significant effect on the core and conduction band, but little effect on the valence band. The band structure calculations indicate that, in this material, the band gap changes from indirect to direct at a pressure of about 25 GPa. In addition, increasing pressure produces a clear curvature in the band structure near the bottom of the conduction band, a behavior consistent with the strong pressure dependence of the transport properties.

Kensaku Kodama et.al. (2014) studied that Non-covalent interactions in bulk CO oxidation on Pt surface were investigated. The role of non-covalent interaction between both non-specifically adsorbed hydrated K+, Li+ and Ba2+ cations (M+) and hydroxyl species (M+-OHad) as well a sunder potentially deposited Cu ad atoms and OHad (Cuupd-OHad) on bulk CO oxidation (COb) is investigated on Pt(111) and Pt(100) in alkaline solutions. The effect of Cuupd-OHad on COboxidation is observed almost at the reversible potential for CO oxidation, signaling that Cuupd-induced adsorption of OHad activates COboxidation at very low over potentials. In contrast, the effect of M+-OHad was found to be strongly dependent on the surface coverage of OHad on Pt; e.g., while no effect is found when the surface is pre-covered by adsorbed CO (COad), a discernable effect is observed on OHad pre-covered Pt surface. The role of non-covalent interactions on CO bulk oxidation on Pt single crystal electrodes in alkaline electrolytes.

Chemical Physics Letter, 2015, 631-632, 6-11DFT study have been performed to examine thenon-covalent interactions among the lighter chalcogenes in a quasi-cyclic systems. The S···O interaction energy has been found to be 6.7kJ/mol calculated at CBS-QB3 level in the gas phase, and stronger than S···S interaction (5.9 kJ/mol). The strength of the interactions of S···X (X = O, S) are less affected with the polarity of solvents compare to that of hydrogen bonds. The AIM analysis reveals that the interactions among the lighter chalcogenes like S···O and S…S are mainly governed by electrostatic effects than hyper conjugative orbital interactions.

WenwuXu et al. (2016) in this work they use computer simulations to explain the variety of crystal orientations observed at interfaces between MgO and Mg when Mg single crystals are oxidized. Using first-principles density functional theory simulations we investigate the interfacial stability of MgO//Mg interfaces, and find that a combination of interfacial chemical bonding. Energy and epitaxial strain stored in the oxide layers can change the relative stability of competing MgO//Mg interfaces. We propose that a combination of the oxygen chemical potential at the interface plane and the epitaxial strain energy stored in the oxide layers is responsible for the differences in observed interfacial crystal orientations–a key insight for the design and development of Mg alloys reinforced by MgO particles.

Kumaraswamy et al., (2017) The new analogs of benzimidazole fused heterocyclic compounds such as triazinane and oxadiazinanes were synthesised by classical amino methylation with different aryl-*N*,*N*′ unsymmetrical thioureas. The anti bacterial activity of triazinane and oxadiazinane compounds have been assessed with zone of inhibition by well diffusion method using a panel of selected gram positive and gram negative bacterial strains and which have showed good activity. The synthesized molecules were subjected to molecular docking studies with two proteins, namely topoisomerase and *DNA* gyrase subunit. The molecular docking studies are supporting the anti-bacterial activity exhibiting high inhibition constant and binding energy.

SinanZhuChi Zhang et al.,(2017) Reduced activation ferritic/martensitic (RAFM) steels are widely applied as structural materials in the nuclear industry. To investigate hydrogen's effect on RAFM steels' elastic properties and the mechanism of that effect, a procedure of first principlessimulationcombinedwithexperimentwasdesigned.Densityfunctionaltheorymodelswe reestablished to simulate RAFM steels' elastic status before and after hydrogen's insertion. Also, experiment was designed to measure the Young's modulus of RAFM steel samples with and without hydrogen charging. Both simulation and experiment showed that the solubility of hydrogen in RAFM steels would decrease the Young's modulus. The effect of hydrogen on RAFM steels' Young's modulus was more significant in water-quenched steels than it was intempering steels. This indicated that defects inside martensite, considered to be hydrogen traps, could decrease the cohesive energy of the matrix and lead to a decrease of the Young's modulus after hydrogen insertion.

FeiKeet.al.,(2018) The structural properties and hydrogen adsorption energy of the fluorinated metal-organic framework (MOF)-801 were evaluated with the help of density functional theory(DFT). The introduction of F atoms is determined to enhance the binding capacity of MOF-801.Fluorine in MOF-801, increases the binding energy of hydrogen where Fluorine atom is directly bonded to Zr in MOF-801. The hydrogen storage capacity becomes larger in fluorinated zirconiummetal-organic framework(MOF-801).

LITERATURE PRECEDENCE

The Watson and Crick model of DNA (1953) depicts DNA as a double helical shape in which the nitrogen bases of one strand make numerous hydrogen bonds with the nitrogen bases of the corresponding strand. 48 Adenine (A), guanine (G), cytosine (C), and thymine are the four nitrogen bases contained in DNA (T). A and G have purine rings, whereas C and T have pyrimidine rings. Out of these four bases, two types of base pairs are commonly found in DNAs*1: C...G (triple hydrogen bond, C-G) and A...T (double hydrogen bond, A-T). It's the Watson-Crick base pairs. However, if we consider the overall possibilities of hydrogen bonding (including both homo- and hetero- patterns) using these four bases, we can find up to 29 possible base pairings. Donohue (1960)49 described 28 of them, and Poltev and Shulyupina recognized the last one (1986). 50 Since the discovery of the DNA structure, the fundamental question has been whether the two base pairs that exist in DNA are the most stable. A variety of works have been devoted to characterizing the structure and stabilization energies of various base pairs using semi-empirical and empirical potentials based on the computer resources available at the time. 50-51 Different analogues of base pairs were created experimentally in order to understand the association propensity of nitrogen base analogues in comparison to Watson-Crick base pairs.

These investigations paved the way for, and later reinforced, the scientific community's conviction that long-range electrostatic interactions in hydrogen bound complexes are undeniably important. The following is a brief history of how the widespread understanding of the relevance of long-range secondary electrostatic interactions has evolved. Previously, it was thought that the primary electrostatic interactions between the hydrogen bond acceptor and donor accounted for the strength of hydrogen bonds. The association constant (Ka) of complex 1, a closer equivalent of the G-C base pair, in chloroform was found to be around 104-105 M-1.52 in the chloroform, the association constant of a comparable complex 2 was

determined to be 1.7 * 105 M-1.53. A detailed examination of the structures of these two complexes reveals that complex 1 contains two primary O...H contacts and one primary N...H interaction, whereas *1 42 other uncommon base pairs, which are rarely encountered, have also been identified in the DNA structure. The most well-known instances are the Hoogsteen base pairs. The N9-H of purines and N1-H of pyrimidines for nitrogen base numbering) were removed for consideration because N9 of purines and N1 of pyrimidines establish covalent connections with the sugar moiety in the DNA structure and are no longer available for hydrogen bonding.

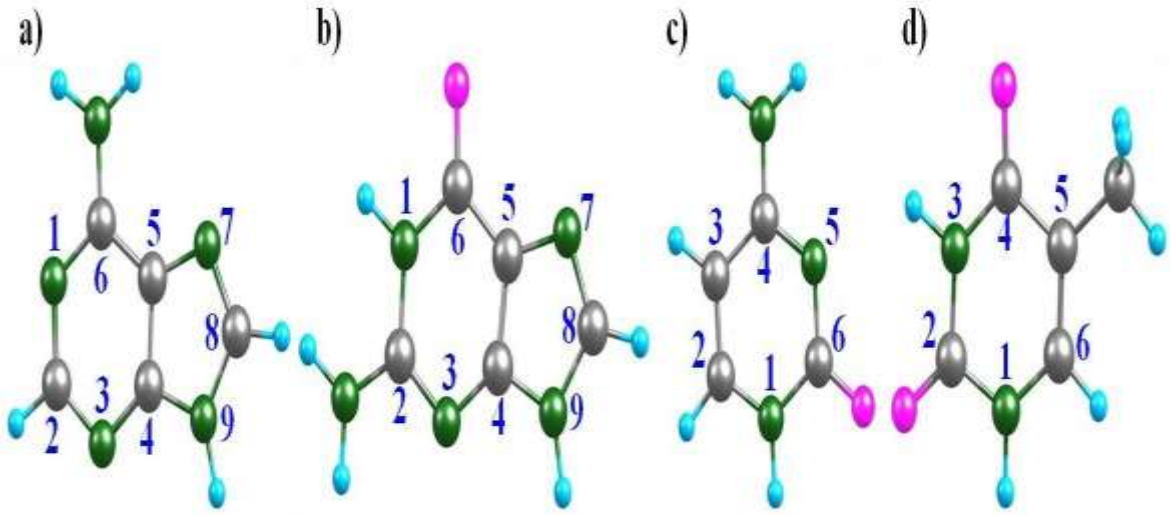

Figure 3: Different Nitrogen bases contained in DNA: adenine, guanine, cytosine, and thymine

METHODOLOGY

I shall used quantum chemical calculations and molecular dynamics simulation for the study of various non-covalent interactions. Methodology use dinmy research work is

(i) Q-Mcalculation (DFT)

(ii) Molecular Electrostatic Potential (MESP) calculation

(i) Density functional theory (DFT)- The density function theory (DFT) model is the most widely used and commercially available model that takes electron correlation into account. Kohn and Sham demonstrated that this method determines potential energy as well as other molecular parameters without solving the wave functions. According to the 53a Hohenberg-Kohn theorem, the external potential is a functional of the ground state density. 53b The potential energy is computed using the electron density in the DFT approach (r). However, there is no precise functional relationship between E and (r), therefore the function must be

estimated rather than derived. The simple expression for potential energy or ground state energy in Kohn- Sham (KS) theory is:

$E=ET+ EV+EJ+EXC$

ET is the kinetic energy term caused by electron motion, EV is the nucleus electron potential energy expressed as a result of nuclear-electron attraction and repulsion between pairs of nuclei, EJ is the classical electron-electron repulsion as well as the Coulomb self-interaction of the electron density, and EXC is the exchange-correlation. The DFT approach incorporates the Pauli principle's exchange interaction as well as electron-electron correlation. The correlation energy is included in the initial DFT approach, which is one of the advantages of DFT over functional-based methods. The exchange correlation (XC) function is a crucial term in the DFT approach because the quality of the exchange-correlation (XC) function determines the accuracy of the DFT calculation. The EXC phrase is written as

$EXC=EX(\rho)+EC(\rho)$

Where EX() stands for exchange functional and EC() stands for correlation functional. Due to its superior performance-to-cost ratio as compared to coupled wave functional theory, the DFT approach is one of the most widely used theories in electronic structure theory. According to the report, the use of DFT approaches has lately increased. 53c The B3LYP method is one of the most common DFT methods for determining the structure of organic compounds. Truhlar has recently developed a number of hybrid-type functionals with the goal of better addressingsome of the known difficult areas of functionals, particularly with weak, noncovalent interactions.

(ii) Elementary Quantum Mechanics the Schrödinger Equation- The basic goal of current quantum mechanics is to solve Erwin Rudolf Josef Alexander Schrödinger's time-dependent non-relativistic Schrödinger equation, which he proposed in 1926. However, if the potential energy of the system is considered to be time independent, the time dependent interactions are frequently not relevant in most chemical problems. As a result, the time independent Schrödinger equation (TISE) is often regarded as the primary equation in current quantum chemistry. The TISE will henceforth be known as the Schrödinger equation (SE). The many body time-independent Schrödinger equation for a system containing n electrons and m nuclei is given by

$$\hat{H}\Psi(\vec{x}_1,\vec{x}_2,\vec{x}_3,...,\vec{x}_n,\vec{r}_1,\vec{r}_2,\vec{r}_3,...,\vec{r}_m)=E\Psi(\vec{x}_1,\vec{x}_2,\vec{x}_3,...,\vec{x}_n,\vec{r}_1,\vec{r}_2,\vec{r}_3,...,\vec{r}_m)$$

where denotes the molecular Hamiltonian operator and and are the coordinates of respective

$$\hat{H}=-\frac{1}{2}\sum_{i=1}^{n}\nabla_i^2-\frac{1}{2}\sum_{a=1}^{m}\frac{\nabla_a^2}{m_a}-\sum_{a=1}^{m}\sum_{i=1}^{n}\frac{Z_a}{r_{ia}}+\sum_{a}^{m}\sum_{b>a}^{m}\frac{Z_aZ_b}{r_{ab}}+\sum_{i=1}^{n}\sum_{j>i}^{n}\frac{1}{r_{ij}}$$

electrons and nuclei, is a many particle wave function for a given system and is a function of the 3n space coordinates and n spin coordinates of electrons and 3m space coordinates of nuclei, and E is the total energy of the system, is also known as the eigenvalue equation, where E is the eigenvalue, and is an eigen function of operator H, which In order to be considered for quantum chemical study, the wave function must meet specific characteristics, which define it as well behaved in atomic units, the Hamiltonian operator is given as, The Hamiltonian's first two terms represent the kinetic energy of electrons and nuclei, respectively. Nuclear-electron attraction, nuclear-nuclear repulsion, and electron-electron repulsion are the final three terms. Indices I and j represent the total number of n electrons, whereas indices a and b represent the total number of m nuclei in the system. Other terms in the equation have their normal meanings. In order to apply QM theory to real-world chemical problems, we must first answer the SE for multi-electron multi-nuclear molecule systems. The exact solution to the SE, however, is limited to a few simple ideal instances, such as a particle in a box, a harmonic oscillator, a stiff rotor, and a hydrogen atom. As a result, approximate approaches have been proposed over the years to make this theory relevant to larger systems. The Born-Oppenheimer approximation is the first to be considered, and it is thought to be a good approximation for stationary point computations.

CONCLUSION

The current study demonstrates a straightforward approach for calculating the electrostatic force (EF) of interaction between two partners in molecular complexes where noncovalent electrostatic interaction is the main factor. More crucially, this study highlights the importance of long-range secondary interactions involving all atoms of one binding partner and all atoms of the other. The paper also emphasises the importance of considering directionality when characterising such interactions and how it may be used to calculate the binding strength of hydrogen bound complexes. It has been demonstrated that the line

connecting the centres of geometries of the frontier atoms of two partners best describes the molecular interactions in multi-hydrogen bound planar complexes. The forces produced by treating atoms in molecules as point charges correspond linearly with the forces obtained by utilising the finite difference approach in EDA analysis. Given the numerous fields of chemistry, material sciences, and biology where long-range electrostatic interactions play a substantial role in defining the overall strength of the contact, the current approach is highly relevant.

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