Daffodil International University

Class Test

Student ID : 241-15-918 Program : ..... Semester : Spring/ Summer/ Year : .....

Course Code : ..... Course Title : ..... Section : K Date : .....

Class Test No. : ..... Signature of the Course Teacher : .....

At last I can say that if I need to deals with electrons then I work with quantum ~~meeean~~ mechanic or dynamic from which type I need to represent the equation ~~meeane~~ mechanicaly or ~~eet~~ classicaly and if I need to work with atom then molicular mechanic or dynamic help me to do this. But molicular dynamis is better than molecular mechanics.

work with only atom, ~~ing~~ ignoring electrom. But mo lare dynamics is more efecent and less time cos co ming from molicular mechanics. Mainly the difference betaeen molicular dynamic and molieular mechanics is how I ~~a~~ want to represent the atom Mechanicaly or classicaly.

(III) Quantum Mechanics:

Quantum mechanics deals with electron. Quantum mechanies majer the electron speed, dencity, charged or not etc. If I need to deeper equation with the electrom then I showed go for quntum mechanies. But it works with electron is very time consuming in Quantum mechanies. Quantum mechanics works with wave fuction equation. Here is the equation:

(IV) Quantum Dynamics:

Quantum dynamics is mainly a quantum mechanis with different type of represectation. Quantum dynamics is also time consamings. It deals with electronic wave using schrodinger equation.

Daffodil International University

Class Test

Student ID : 241-15-218 Program : CSE Semester : Spring/ Summer/ Year : 2024

Course Code : 115 Course Title : ICBC Section : K Date : 04/03/24

Class Test No. : 02 Signature of the Course Teacher :

Q1 Compare and Contrasting the efficacy, speed, accuracy and computational resources required for employing molecular mechanics, molicular dynamics, quantum mechanics and quantum dynamics, is bellow:

① Molecular Mechanics:

Molecular mechanics equation is use to solve the classical physicas. It treats atoms sring, bonds, and it ignored electorns. If I showed not need to deep calculation with electrons and calculate atom in mechanicaly then molecular Mechaniss help me to do it. It easume that the sum of total energy potential energy is cosm comes from attractive force and repi give force between atom. Here is the equation of molicular mechanics: $E = EA + EB + ED + ENB^*$

② Molecular dynamics:

Molecular dynamics is the mdecular mechanics equation to mimic the movement of a atom. It also

241-15-918
66-K

Daffodil International University

Faculty of Science & Information Technology

Quiz 2, Spring 2024

Course Code: CSE115

Course Title: Introduction to Chemistry and Biology for Computation

Level: 1 **Term: 1** **Batch:66**

Time: 40 minutes **Marks: 15**

Answer ALL Questions

[The figures in the right margin indicate the full marks and corresponding course outcomes, program outcomes. All portions of each question must be answered sequentially.]

1.	Imagine you're exploring the intricacies of DNA replication while unraveling the structural nuances of adenine and uracil, essential nucleobases in RNA. **Define** the unique structures of Adenine (A), Cytosine (C) contribute to the fidelity of genetic information transfer and the dynamic process of DNA replication. **Explain** the DNA replication process?	**[5]**	**CO1** **PO2** **L1**
2.	Imagine you are tasked with simulating the behavior of a complex biomolecular system, such as a protein-ligand interaction crucial for drug discovery. The system involves significant conformational changes and interactions at the atomic level. **Compare and contrast** the efficacy, speed, accuracy, and computational resources required for employing molecular mechanics, molecular dynamics, quantum mechanics, and quantum dynamics approaches to study this system. Which method(s) would you recommend based on the balance of these factors? How do the methods differ in capturing essential features of the system dynamics and providing insights for potential drug design or other applications?	**[10]**	**CO2** **PO4** **L2**