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The Investigation of Different Properties of Si_5O_{10} Nano Structure as a Carrier for particles and drugs: A Theoretical Study

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Abstract

In the search for new drug and medication discovery, especially related to drug-receptor interaction, the importance of interaction among researchers is essential, either within the same room or dispersed throughout the world. An architecture that uses concepts of Distributed Multiuser Virtual Reality, Computer-Supported Collaborative Work, and world-wide network communication techniques for creating a high performance system that allows real-time interaction among various geographically dispersed research groups studying molecular visualization and using hardware systems ranging from desktop to immersive systems as caves is presented.

Density functional theory calculations are carried out to study the effects of binding some atoms and ions to Si_5O_{10} cave. Binding energies, NBO, Charge Mullikan population parameters and HOMO- LUMO gap energy were calculated. Results from binding energies indicate that it is possible thermodynamically to bind some molecules and ions to Si_5O_{10} cave. The values of HOMO, LUMO and HOMO–LUMO Gap energies are calculation for molecules and ions to Si_5O_{10} cave using M062X method and 6-31G basis set. From HOMO–LUMO Gap calculation, it can be seen that HOMO- LUMO Gap energy of decrease in the order: Si_5O_{10} cave to H^+ > Si_5O_{10} cave to He^{2+}> Si_5O_{10} cave to D_2> Si_5O_{10} cave to H_2 and by decreasing of HOMO- LUMO Gap energy, would be more stable compound. So, H_2 beside Si_5O_{10} cave can act better as an electron donor. Additionally, NBO, Charge Mullikan population parameters have been investigated. We arrive at the prediction that the Si_5O_{10} can be implemented as a novel material for some molecules, ions and drug delivery applications.*

Keyword: DFT, Cave, some atoms and ions, Binding and Electromagnetic parameters.

1. Introduction and Methodology

In Medicinal Chemistry, it is needed to have great knowledge in organic chemistry, pharmacology, physics, biology, medicine, and docking studies supported by computer, everything at once. It means having a multidisciplinary environment, and it almost never happens in a single Department, Campus or even in cities. Therefore, there is a great need of creating a collaborative atmosphere among geographically separated research groups so they can research structures, properties and molecular dynamics, quickly, without necessarily need to be together in person.

Over 40 years, the attention is focused on the development of drug delivery systems [1-3]. These systems are designed to reduce the frequency of use, increased drug efficacy and reduced side effects. Polymers [4, 5] and caves used as atom transfer and drug delivery systems. In recent years, significant developments have been made in using caves biomedical polymers as carriers for targeted delivery of drugs, proteins and growth factors. The nature of the networks, pore sizes, sustainability and response to external stimuli are the most important features of these networks. By combatting and eliminating the clinical and pharmacological limitations of caves it is possible to make more specific and appropriate products. In this paper, we describe some of the caves. The cave used in this study containing 5 Si and 10 O atoms. There were covalent bonds between atoms. Covalent bond is stronger than non-covalent bonds and provides very good mechanical stability. Here, we have presented a theoretical study on the different properties of cave to some atoms in the framework of a tight-binding approach. For example, one of the main points in the study of such systems concerns the internal magnetic structure of the cave as a function of their shape and size. The magnetic cave -objects have been deeply investigated during the last decades. Besides, the basic scientific interest in the magnetic properties of these systems, there is evidence that they might be used in the production of new technological application [6].