STABILITY OF IONIZED AIR USING DENSITY FUNCTIONAL THEORY (DFT) FOR HIGH VOLTAGE ENGINEERING

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STABILITY OF IONIZED AIR USING DENSITY FUNCTIONAL THEORY (DFT) FOR HIGH VOLTAGE ENGINEERING

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ABSTRACT

In high voltage engineering, air is the one insulation gas that can ionized cause by electrical discharge. Air consisted of many gases such as O_2, N_2, CO_2, H_2, etc. In order to study the characteristic of the insulation gas, we can apply density functional theory (DFT) to determine gas ionization level such as charge distribution and excitation energy. These data are shown the stability of molecule gas when ionization process occure cause by electrical discharge, ultraviolet light, etc. For application on ozone production by electrical discharge, the oxygen atom can transform to ozone need energy above the stabiity excitation energy of oxygen.

INTRODUCTION

Generally, the high voltage engineering is focused on electrical discharge on the insulation dielectric in the form solid, liquid and gas. Base on our previous research, computational approach can be used to study the air failure in the high voltage which can be utilized to generate ozone from the ionization process of the oxygen atoms [1]. The ionization process has been checked using homo-lumo application. In this research, density functional theory (DFT) has been developed as reliable and effective approach for the computer simulation of molecular structure and also to measure the energy for chemical reaction. DFT is also can be used to search the efficiency and acuracy of the molecular properties, such as electronegativity, chemical potential and affinities [3]. The molecular properties of can be accurately described and calculated by manipulating the electron density and its fundamental quantity.

RESEARCH METHODOLOGY

Preparation of Molecular Gases

Preparation of molecular gases i.e. O_2, N_2, H_2, CO and CO_2 is beginned with skecthed of each molecular gases using ChemBioDraw ultra 13.0 for then it should save it in mdl. mol format. for then imported it into the Gaussian software.

DensityFunctional Theory (DFT)

The initial structure of each gas O_2, N_2, H_2, CO and CO_2 are needed to obtain, density functional theory (DFT) is urgently needed to optimize the stability of these gases. DFT was runned using Gaussian 09 software with 6-311G/B3YLP was selected as basis set. Basis set is shape of atomic orbital that explained using wave function. TD-SCF was used as method to perform the Gaussian [4]. Stability of the calculation was explored the stability of the wavefunction computed for a molecular system. The stability of SCF solution for unknown systems should always be tested. The consideration for stability of unknown systems should be apply and may be tested in calculation using DFT methods as well.

Results and Disscussion

Single particle are described about molecules or atom or also described how the chemical bonding between each atom to make a molecule. In this study, density functional theory (DFT) was applied to check the stability of gases and also to study shock induced process because they involve spatial and temporal scales that go beyond those attainable at the atomistic level. The stability of each gas such as N_2,O_2, CO, CO_2, and H_2. base on the DFT calcution we will know charge distribution and excitation energy [5]. DFT calculation provides the energy of ionization potential for these gas elements.

Molecule N_2

The gas N_2 is seems to be stable at the wave length 89.17 nm, based on DFT calculation for the best pose selected with the following results; energy of excitation of 89.17 eV, energy for the ionization process of 108.98 from orbital eight of -0.13492 to orbital seven of -0.42842. The ionization process of molecule N_2 is depicted in Figure 1.

Molecule consisted of atoms and atoms consisted of electrons. Excitation of each electron in orbital atoms cause the ionization process. The ionization process is stable if the range

energy between two orbital less than 0.9 eV [6]. For gas N_2, there are two electrons was jumped from orbital eight into orbital seven with the range energy of 0.56334 eV. It is indicated that gas N_2 is stable.

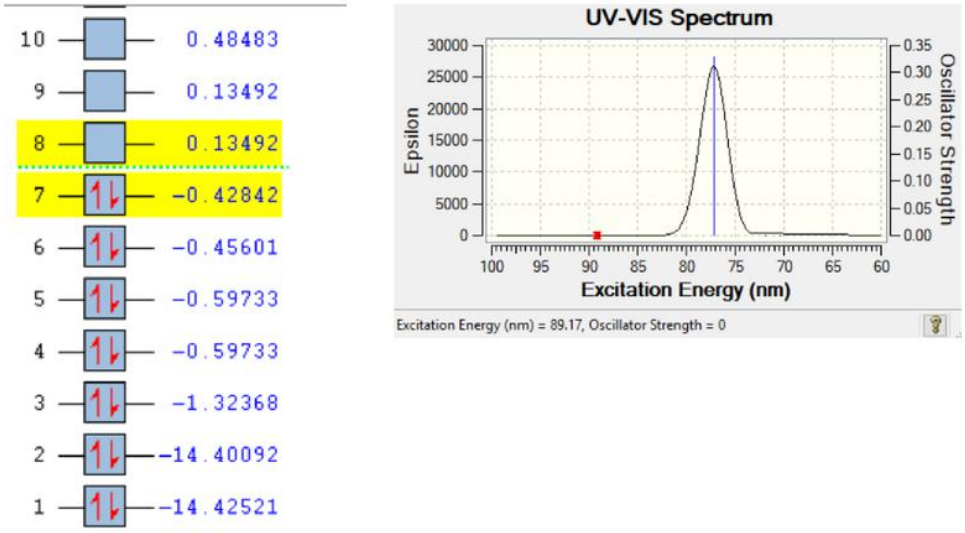


Figure 1. Ionization process of gas N_2

Molecule O_2

Generally, DFT can be defined as method for computational quantum mechanical modelling used in physic, chemistry or material science for investigating the properties of electron in a system, hence the name density functional theory comes from the use of functionals of the electron density.

Like gas N_2, ionization of molecule O_2 is looks stable since the excitation energy of -395143 eV with the wave length of 395143 nm, the best pose selected with the following results; energy for the ionization process of 108.98 au from orbital nine of 0.01523 to orbital eight of -0.05553. The ionization process of molecule O_2 is presented in Figure 2. Stability of gas O_2 is shown with there are two electrons was jumped from orbital nine into orbital eight with the range energy of 0.07053 eV.

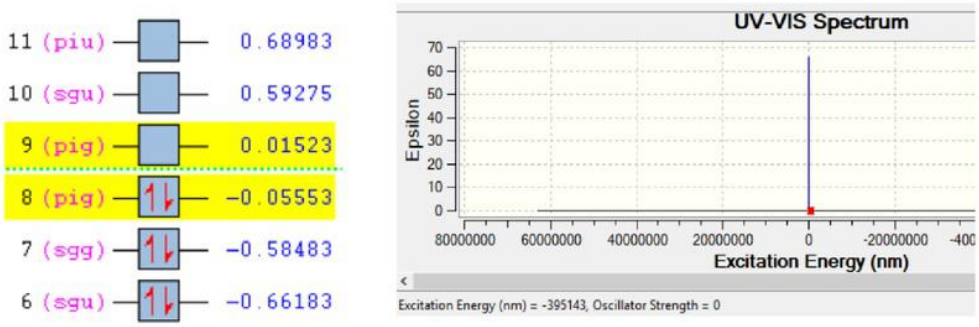


Figure 2. Ionization proses of molecule O_2

Molecule H_2

The stability of molecule H_2 is also checked using the same way like molecule O_2 and N_2. Base on DFT calculation, it come out with the excitation energy of 88,8 eV at the wave length 88.8 nm. Two electrons were jumped from orbital two into orbital one with the energy of 0.49436 eV. Figure 3 is presented the ionization process of molecule H_2.

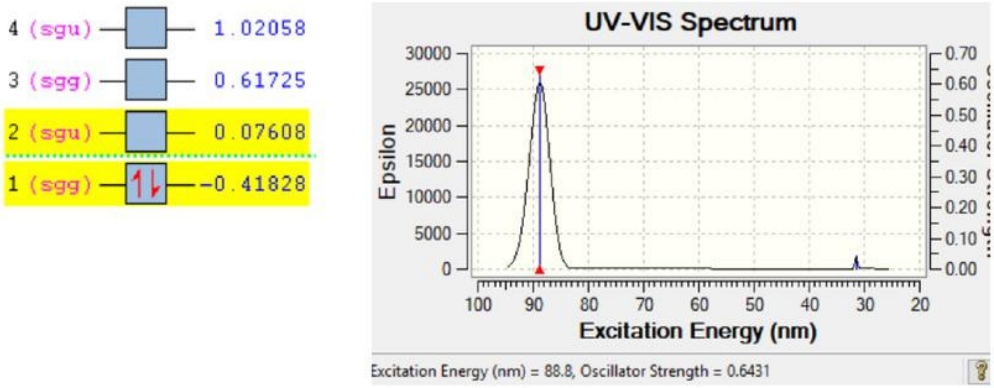
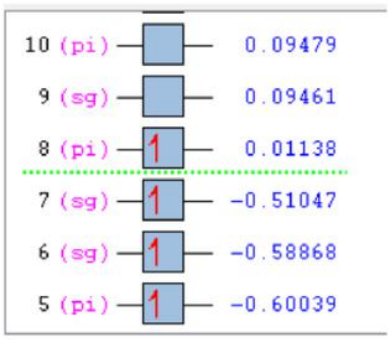


Figure 3. Ionization process of molecule H_2

Molecule CO

Stability of molecule CO was checked using DFT. The first principles of DFT is to carried out the structural stability and also the electronic properties of a molecule. Base on DFT

calculation, gas CO has the excitation energy of 167782 eV. Only one electron was excitited from orbital eight into orbital seven with the energy of 0.52185 eV. The process of elctron excitation for molecule CO is depicted in Figure 4.



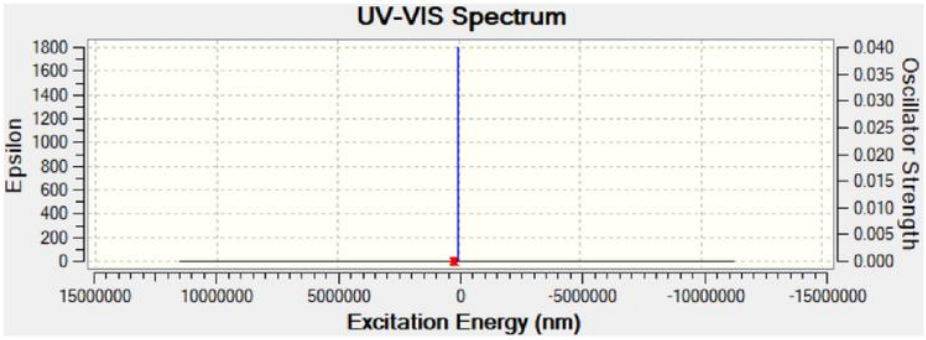
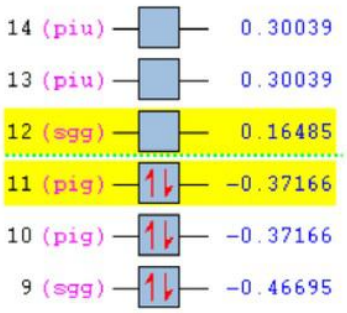


Figure 4. Ionization process of molecule CO

Molecule CO_2

DFT determined the stability of molecule CO_2. Base on the DFT simulation, molecule gas CO_2 is also looks stable with the exitation energy of 96.13 eV. There are two electron were excitited from orbital eleven into orbital ten with the energy of 0.53651 eV. Figure 5 is presented the ionization process of molecule CO_2.



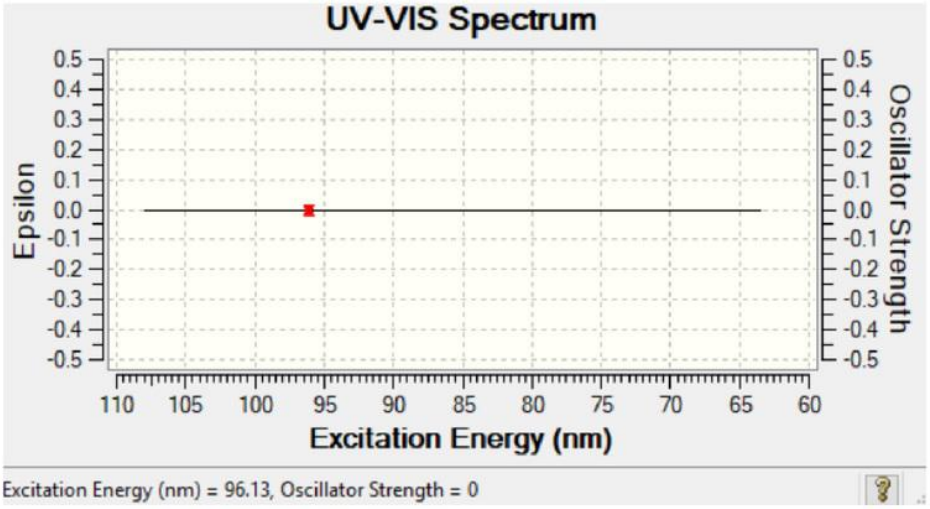


Figure 5. The ionization process of molecule CO_2

Conclusion

There are several conclusions that can be concluded base on this research:

1. Density functional theory (DFT) has been developed as reliable and effective approach for the computer simulation of molecular structure.
2. The ionization process is stable if the range energy between two orbital less than 0.9 eV.
3. Gas molecule N_2, O_2, H_2, CO and CO_2 is stable with the excititation energy of 0.01523 eV, 0.56334 eV, 0.49436 eV, 0.52185 eV, 0.53651 eV

Acknowledgement

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