

CHAPTER I

INTRODUCTION

I.1 Research Background

Electronic structure determines all physical properties of materials. As the name says, the electronic structure is the dynamics of electrons in the materials. Quantum mechanics states that the dynamics of electron can be represented as the orbital wave function (ψ_i) and its corresponding energy (e_i). For example, some molecules tend to be in their ionic charge state because one valence electron is in the unstable orbital – as it has been proved by Febriana ([Feb19]). Other molecules may be in the neutral charge state, but it tends to react with other molecule because of its high reactivity (radical molecules) – as it has been proved by Munir ([Mun19]).

The electronic structure is the solution to the Schrödinger Equation. The Schrödinger equation describes each system differently. Simple systems, like the infinite square well potential and the harmonic oscillator potential, have simple solution. However, when it comes to the atomic system, the exact solution to the Schrödinger equation only comes from the one electron atom: Hydrogen atom. On this systems, the potential energy only comes from the interaction between the nuclei and the electron. The solution to the Schrödinger equation for systems with more than one electrons need some approximation ([ABW13]). In many-electron systems, there are too many interactions– nuclei-electron and each electron-electron interactions. These electron-electron interactions correlate one and another in each of their Schrödinger equations. Those equations have to solved simultaneously, which is not supported by any mathematical tools.

The approximations to the Schrödinger equation approximate the electron-

electron interaction in some way. The examples mentioned earlier ([Feb19] and [Mun19]) approximate the Schrödinger equation with Density Functional Theory (DFT) to calculate the electronic structure of their molecules of interest. Generally, DFT approximate the electron-electron interaction as the electron density. The electron density is treated in some way to form the electronic structures that gives the most negative total electronic energy (E). Somehow to achieve this, the electronic structures is virtual—have no physical meaning. Another common approximation for the electron-electron interaction is Hartree-Fock (HF). Hartree-Fock calculation consider the electron-electron interaction only in average sense [FF96]. Both HF and DFT derive the electronic structure directly with no inclusion of experimental data. These kind of computations are the *ab-initio* calculation. It is Latin for "from the beginning" ([You01, Chp.3]). HF and DFT are numerical method and require them to be integrated with computer program like Gaussian and Quantum Espresso. With adequate computer resource, the HF and DFT calculation could be run simply. They have been used widely in field of quantum engineering and quantum chemistry.

For molecular case, the approximation to the Schrödinger equation could be done in a more simple way: the Molecular Orbital Theory (MOT). Instead of approximate the electron-electron interaction, MOT consider the electronic structure of a molecule as the linear combination of the orbitals of its constituent atoms. To maintain its physical meaning, these atomic orbital could be formed by some experimental data. The molecular orbital from these "meaningful" atomic orbital should also has physical meaning. Not like two former approximations, MOT calculation that derive the orbital is analytical. This made MOT calculation is basically easier than HF and DFT.

Motivation of this research comes from the fact that electronic structure from MOT calculation are undoubted. In another hand, the electronic structure from DFT calculation used in [Feb19] and [Mun19] are virtual. This research evaluate the electronic structure from both *ab-initio* calculations de-

scribed earlier based on MOT point of view. Along with it, two physical properties are also evaluated. They are the electron population and the dipole moment. Both of them are derived directly from the electronic structure of each molecule. Molecules of interest of this research are five diatomic molecules mentioned on Subchapter I.4 "Problem Limitation" (page 3). Each of them is unique, either from the orbital type of orbital of the constituent atom or the electron arrangement on the molecules.

I.2 Problem Statement

How MOT evaluate the *ab-initio* calculated electronic structure from HF and DFT calculation?

I.3 Goal

Using MOT to interpret the *ab-initio* calculated orbital wave function, its corresponding energy, and two physical quantities derived from them: ionization potential and dipole moment of five simple molecules.

I.4 Problem Limitation

There are four limitations of problem for this research.

1. The simple molecules are
 - (a) H₂
 - (b) HLi
 - (c) HBe
 - (d) HO
 - (e) HF
2. DFT calculations are run using exchange-correlation functional B3LYP.
3. Basis set on HF and DFT calculations are
 - (a) STO-3G

- (b) 3-21G
- (c) 6-31G
- (d) 6-31G(d,p).

4. The MOT calculation only consider two orbital interaction.

I.5 Outcome

Interpreting electronic structure from HF and DFT calculation with orbital interaction approach (MOT), which will be done on this research, will bring an advanced and unique understanding about them. The results of this research will be a good consideration for anyone either to use or not use the electronic structure resulting from HF and DFT calculations.