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Modeling of Ionization Energy of Elements Using Hartree-Fock Method: An Introduction to Computational Quantum Chemistry for Undergraduate Students

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Abstract The periodic properties of elements are central to the concept of chemistry and are deeply depending on the electron configuration of atoms. Among the common periodic properties such as atomic radii, electronegativity, electron affinity, the ionization energy of elements gives a clear trend in periodicity. Here, we present a classroom activity, mainly for undergraduate students, to simulate first ionization energy as an important periodic property of elements (up to xenon atom). A set of Hartree-Fock calculations were performed with Gaussian 03 suit of programs and the results have been compared with that of the experimental values. While comparing the experimental and calculated values, we have stressed the role of central-field approximation in the HF theory, important features of Slater type orbitals near the nucleus and the significance of electron correlation in multi-electron systems. Some suggestions for improvement of the results are also discussed.

Keywords: *periodic properties, computational chemistry, Hartree-Fock, ionization energy, atomic structure*

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1. Introduction

The modern periodic table is one of the most perfectly arranged data at our scientific disposal and a fundamental source of information for a chemist [1,2]. For centuries, chemists had been working to shed light on the systematic arrangement of the elements [3]. The similarities in numerous physical and chemical properties of elements led to the concept of periodicity of elements. However, the arrangement of elements in the modern periodic table is solely based on the electron configuration of atoms. Here, as a *first time* computational chemistry laboratory activity to undergraduate students, we simulated the periodicity of first ionization energy (IE) of elements with Gaussian electronic structure program [4]. The calculated ionization energies were compared against experimental values and found a semi-quantitaive agreement between the theory and the experiment.

The motivation to write this article is the following. In general, *ab initio* computational chemistry is introduced to under-graduate curriculum (chemistry major) by introducing Hartre-Fock (HF) method and, nowadays, often accompanied with density functional theory. As an immediate application to these methods, most of the text books [5,6,7] treat molecular systems and calculates the properties such as equilibrium structure, molecular energy levels, shapes of molecular orbitals etc. However to fully understand the results from these calculations, the students are expected to have a good knowledge in molecular orbital (MO) theory along with the group theory (for instance, to analyze molecular orbitals, or bonding). In fact, almost every molecular quantum chemistry package is heavily depending on the symmetry-adapted subroutines since it substantially speed-up the *ab initio* calculations. But in this computational work, students with no knowledge of these theories can participate as well and learn the basic terms or concepts of computational chemistry (such as the idea of a basis set, difference between Slater type orbitals (STO) and Gaussian type orbitals (GTO), significance of electron correlation etc). Since these single-atom calculations take only a short time (typically less than two minutes for each atom on a standard 2 GHz PC), every student in the class can do this computational work independently. Though the students are not expected to have a prior knowledge in Gaussian program, we strongly recommend that the teacher/demonstrator should teach them some basic key-words as well as the structure of the Gaussian input/output file before the calculations (See the supplementary