On the Development of a New Computational Chemistry Software

Han Ung Lee, Hayan Lee and Wilfredo Credo Chung*

Department of Chemistry, De La Salle University – Manila, 2401 Taft Avenue, Manila, 1004 Philippines
Corresponding Author: email wilfredo.chung@dlsu.edu.ph

Abstract: FIESTA—the Filipino Initiative on Electronic Structure Theory and Applications—a new computational chemistry software is developed. The new software is capable of doing ground-state self-consistent field (SCF) single-point restricted Hartree-Fock (RHF) calculation of polyelectronic and polyatomic systems using the Slater-type orbital basis set STO-3G. The new program implements well-known quantum mechanical theories for practical calculations. FIESTA is written using two programming languages, namely C and FORTRAN. It is accurate and user-friendly. It runs efficiently under the Linux operating system and is able to reproduce the energies calculated using well-established standard quantum chemical software products Gaussian, Firefly and Molpro. To our knowledge, FIESTA is the first and only molecular modeling software developed in the Philippines to date. The software will be extended to calculate the properties of systems such as atoms, molecules, ions and formula units using more sophisticated basis sets and quantum mechanical techniques.

Key Words: computational chemistry; ab initio calculation; Hartree-Fock theory; self-consistent field