**An Overview of Quantum Chemistry Calculation**

Seol Ryu

Chosun university, Department of Chemistry,

309 Pilmun-daero, Dong-gu Gwangju 501-759

A brief introduction to quantum chemistry calculations will be provided for description of molecular systems where not only Coulomb and exchange interactions but also electron correlation effects should be taken into account. Differences between the wavefunction-based ab inito and density functional theories will be explained in detail. Very simple examples and calculation results employing one of the most popular density functionals, i.e., B3LYP, will be given to show how much a density functional method can accomplish. In the examples, structures of mono- and dihydrated adenine dimers and their cations are calculated using B3LYP functional with the 6-31+G(d,p) basis set in order to help understand photofragmentation experiments of hydrated adenine dimmers. Several important pathways leading to the major fragmentation product, protonated adenine ion (AH+), thermodynamically at minimum costs are investigated at the ground-state electronic potential surface of hydrated adenine dimer cations.