Hartree-Fock

We started by learning **Hartree-Fock** method, the bare bone for the successful methods that came after. Hartree-Fock theory is an ab initio **Quantum Chemistry** calculation method. It is an approximating method that writes the wavefunction using spin orbitals basis set and the ground state of the Slater determinant as the trial wavefunction. After learning Hartree-Fock, we saw how the basis sets affect the accuracy of our solution. However, even with taking the infinite limit of the basis set, which will yield the exact **Theory solution**, this solution will not represent the true energy of our system. That is because the theory itself is flawed and is missing important information.

Post-Hartree-Fock

The main issue with Hartree-Fock is that it completely neglects **Electron Correlation** completely, which led to a huge deviation from experimental data. So, new models were needed and new methods came out trying to introduce electron correlation. **Configuration Interaction** method was one of the first to attempt to introduce the electron correlation, it was only applicable to systems with a small number of electrons so we needed to truncate it; which introduced a new issue of size consistency. Another method attempted to add the electron correlation as a **Perturbation** to the energy. However, it was not variational nor did including higher terms ensure better results. Then, **Coupled Cluster Theory** Came and introduced a highly accurate electron correlation energy estimation. However, it has the highest computational cost as it scales with N^6. These methods along with HF can estimate HF energy, optimize the geometry, find ionization and electrostatic potentials, and determine molecular orbitals for small systems as they cost the most.

Classical Calculations

After learning quantum chemistry calculations using HF and post-HF methods, we are now back with **Molecular Mechanics and Dynamics**. Which is essentially neglecting the quantum nature of the system and treating it classically. The huge advantage of this is that we can simulate and calculate the properties of a huge number of atoms, which is not possible using quantum chemistry methods. Molecular mechanics methods are used to describe large systems like proteins using empirical formulas and subdividing atoms into categories that share the same properties to lower the computational cost even more. Molecular dynamics methods are essentially aimed to find the equation of motion using newton's equations or any other method -Like Lagrange's equation-. The **Monte Carlo method** is used in MD, which is a genius method aimed to find the minima in the potential energy surface, it can use the internal coordinates to perform the search and can jump potential barriers easily -even none-physically-.

Personal Opinion

Finally, I want to say a couple of words about my personal opinion on the course. This course was AMAZING, I did not expect it to be this well put and this informative. At first, I was thinking of dropping it because I got stuck trying to learn the concepts and thought that this is not for me as a physics student. Oh was I so wrong! I learned so much which I stated briefly, and If I had more space I would keep talking and detailing. The instructor did put a great effort into this course to come out this good, and I really am grateful for taking the course.