Goals:

- 1. Understand the basic principles of quantum mechanics.
- 2. Understand the principles of LCAO-MO and Hartree-Fock approximation
- 3. Familiar with the concept of density functional theory
- 4. Familiar the commonly used basis sets
- 5. Understand the concept of electron correlation and methods that address the problem
- 6. Capable of use Gaussian to study molecular properties