Density Functional Theory

I) Lectures:

a) Density-Functional-Theories (7-09-2016, 10:30-12:00)
Orbital-free FDT
Kohn-Sham DFT
Generalized Kohn-Sham (adiabatic connection)
Multi-configurational DFT

b) Density functional approximations (7-09-2016, 14:00-15:30)
LDA,GGA, meta-GGA, hybrid functionals, range-separated functionals

II) Exercises (8-09-2016, 14:00-15:00)

a) We will use Gausaian09 and Molden (or other software) for visualization of the orbitals

b) The molecule : (uracil)

c) Method DFT(B3LYP) and HF

d) Geometry:
- If the students know Gaussian and internal coordinates than they will construct the geometry themselves if know the input will be given and explained
- Basis sets: at least three different of increasing size

1) Exercise I:
- Perform B3LYP calculations for each basis sets
- Analyze the convergence (how many steps, how long the calculations take, what is the size of the basis set)

2) Exercise II (further analysis of the results obtained in I):
- Discuss the absolute energies obtained using basis sets of increasing size as illustration for variation principle
- Visualize the orbitals from HF and from DFT(B3LYP) , discuss similarities and differences
- Discuss the orbital energies and HOMO-LUMO gaps obtained using HF and DFT(B3LYP) and the considered (at least) three basis sets.

3) Exercise III (optional)
Verification of the eigenvalue theorem.
Compare orbital energies of HOMO with the ionization potential calculated as the difference of total energies obtained from two DFT(B3LYP) calculations for N and N-1 electrons (additional runs needed).