# **Total energy of the system**

*Organize*[*SCF cycle*](https://www.dsedu.org/courses/dft/scf)*to solve KS equation. Use analytical solution of Schrödinger equation as a starting point and use SCF mixing parameter  to find self-consistent solution. Plot the radial wavefunction calculated numerically and compare with analytical solution. Plot nucleus potential, e-e potential, XC potential. Find self-interaction error.*

Now you can combine all studied modules in Tasks 1-10 to organize your DFT program. Follow the following scheme and suggestions.

![图示

AI 生成的内容可能不正确。]()

1. Set , , , and calculate mesh , .
2. Calculate analytical solution ,  (see Eq. (6) from [Task 1)](https://www.dsedu.org/courses/dft/h-atom), and use it as a first approximation to the solution of the Kohn-Sham (KS) equation , .
3. Calculate nuclear potential  (Eq. (2) in [Task 2](https://www.dsedu.org/courses/dft/ks)). Using procedure *Vcoul*from [Task 7](https://www.dsedu.org/courses/dft/veef) calculate e-e potential  corresponding to . Using procedure from [Task 3](https://www.dsedu.org/courses/dft/xc) calculate XC potential corresponding to . Calculate KS potential  as a sum of , , and .
4. Solve KS equation using *Diff*procedure from [Task 8](https://www.dsedu.org/courses/dft/ks_eigenvector) to get the radial wave function  .
5. Calculate norm of the radial wave function  and renormalize the solution .
6. Using procedure *Vcoul*from [Task 7](https://www.dsedu.org/courses/dft/veef) calculate e-e potential  corresponding to . Using procedure from [Task 3](https://www.dsedu.org/courses/dft/xc) calculate XC potential corresponding to . Calculate KS potential  as a sum of , , and .
7. Set the KS potential for next iteration as a mix of potentials and using : .
8. Using procedure *Energy* from [Task 9](https://www.dsedu.org/courses/dft/ks_eigenvalue) calculate KS energy  corresponding to .
9. Check the difference , if this difference is greater than , then print energy , norm of the wave function for current iteration, and set , , and  as initial values for next iteration, go to **step 5**, and make additional SCF iteration to get new values of  , , and , and so on until you reach self-consistent convergence. Set maximum number of iterations to . Check number of iterations, if number of iterations reached , then print error message and stop the program. If the SCF error less that , then you reach SCF convergence, go to the next step.
10. Calculate the total electronic energy  of the system (see [Task 10](https://www.dsedu.org/courses/dft/tot_energy)).
11. Print solution , KS energy , total electronic energy , e-e potential, nuclear potential, XC potential, and total KS potential.
12. Plot the radial wave function  and compare it with analytical solution . Plot e-e potential, nuclear potential, XC potential, and total KS potential.
13. Change  to 0.2, 0.3, ... and repeat the whole procedure from the beginning to see how SCF cycle works.