Exam: Short report + presentation

Date: Monday December 15

Format

The exam consists of writing a short report on a topic within density functional theory (a few pages or as much as you need) and a presentation of 10-15 minutes (on December 15) on the same topic. The work can be done alone or with 2 persons (in that case each will need to give part of the presentation). The report should be handed in by Thursday december 11.

Suggested topics

The topics can be suggested by yourself. Depending on your taste it the topic can range from an applied to a fundamental theoretical issue with density-functional theory. One option is to study in a bit more detail some of the topics in this course. A few suggestions are:

- The local density approximation and its performance
- The gradient expansion, when does it work?
- The generalized gradient expansion, advantages and disadvantages
- v-representability in density functional theory
- Density functional theory for superconductors
- (Time-dependent) current-density functional theory
- Performance of density functional theory in chemistry (comparison to non-DFT methods)
- Exchange- and correlation holes in many-body systems
- The use of Kohn-Sham orbitals in chemistry.
- Memory in time-dependent density-functional theory
- Correlation functionals in DFT
- van der Waals interactions in density functional theory
- Relativistic density-functional theory
- Quantum transport with time-dependent density functional theory
- Kohn-Sham potentials and eigenvalues
- ..

- .. or something that you can suggest yourself

For further information and background literature you can always ask me for suggestions. The review papers by Perdew and Kurth and by von Barth are useful sources for references as well.

Good luck,
Robert