Density functional theory and its applications in nanoscience, FYSM540

Contact hours 48 h (lectures: 24 h, discussion and homework exercise clinic: 24 h)
Fall 2008, weeks 40 – 51, Mondays 10-12 and 13-15, 29.9. -, NSC lecture room YN121
Target audience: doctoral students, advanced masters students, post docs
Credit: 8 ECTS,   project work / presentation
Lecturers: Robert van Leeuwen, Hannu Häkkinen, Karoliina Honkala
Course coordinator: Hannu Häkkinen
Primary material: lecture notes
Additional literature: reviews, parts of the following books:
R.M.Dreizler and E.K.U.Gross. ¨Density Functional Theory¨ (Springer 1990), R.G.Parr
and W.Yang, ¨Density Functional Theory¨ , M.A.L.Marques, C.A.Ullrich, F.Nogueira,
A.Rubio and E.K.U.Gross (eds.), ¨Time-Dependent Density Functional Theory¨, Lectures
Notes in Physics Vol.706 (Springer, 2006)
Web page: http://users.jyu.fi/~hahakkin/opetus/FYSM540-2008/

Content:
I. Ground-state formalism (6 lectures): the many-body problem of electron gas, exchange
and correlation, Hartree-Fock approximation, Hohenberg-Kohn theorem, Kohn-Sham
method, gradient approximations to the exchange-correlation functional, exact exchange,
spin-density extension
II. Time-dependent formalism (3 lectures): Runge-Gross formalism, linear response,
time evolution, time-dependent exchange-correlation functionals
III. Applications (3 lectures): electronic and optical properties of nanoparticles, electron
transport in nanowires, catalytic metal particles and surfaces