student summaries and exam question suggestions
DFT (part 2)

These pages contain student summaries for the module **DFT (part 2)**, *as well as student suggestions for exam questions on this module. You can use these pages as a study help for this module. The summaries can help you to see the highlights of this module from different points of view. The questions can challenge you to think about the content. If you take the exam, then some of the questions suggested this year will be included in the exam. The contributions suggested this year are* are printed in color. *The ones in black were contributed in previous years.*

1. student summaries

- Exchange correlation functional and the numerical methods to solve DFT.
- The properties of a quantum system can be fully understood using the density. The Kohn-Sham equations show how this can be done. To solve this equation, the exchange-correlation functional needs to be found.
- The concept of the Kohn Sham equations and the exchange correlation functional
- The convergence testing is an important aspect in finding the cirrect value for any parameter that you want to calculate on your material.
- The two central theorems, and its relation to the Kohn-Sham equations. What is the exchange and correlation functional and why is needed.
- DFT is a computational method. It does not calculate wave functions but is uses electron density wich contains all the information of the structure. The calculations can't be done analytically, so must be done numerical by using computational algorithms and approximations.
- What the importance of the exchange correlation function is, what information it contains and how the presence of this function sets DFT apart from other methodes of solving the schrodinger equation numerically.
- First key insight is that the ground state electron density uniquely maps to an external energy. The 2nd HK-theorem does explicitly stand by itself because it does provide the understanding that the variational principle applies to the densities, which the 1st theorem does not explain.
- The amazing implications of the first Hohnberg Kohn theorem: both its meaning as well as its consequences.
- Hohenberg-Koh, theorems, Kohn-Sham equation, exchange-correlation functional, Jacob's ladder, numerical solution methods.
- Hartee Fork vs DFT
- The two Hohenberg-Kohn theorems and why the make DFT possible. Then the Kohn-Sham equations and how they are used to obtain a solution.
- The information about both Hohenberg-Kohn theorems. The exchange-correlation functional
- From the first HK theorem we know that the ground state electron density uniquely determines all observable properties of the system. From the second HK theorem we know that the ground state energy functional is minimized when the ground state electron density is used as input. The Kohn Sham scheme is a practical method of implementing DFT. It turns our many body problem into the computationally simple problem of solving a set of independent particle equations. We need to make sure all our DFT calculations have converged, convergence of the hydrostatic pressure is a good indicator of convergence.
- The HK1 and HK2 theorems define the existence and the form of the Exchange Correlation Functional. The pseudo potential-Plain wave method helps to reduce the complexity of the problem but smoothening the potential near the nuclei.

- Meaning of first and second HK-theorems, basic meaning of "self-consistency problem", understanding what is "correlation" with help of solar system analogue
- consecuences of both theorems and the concepts of exchange and correlation
- The role of the exchange-correlation potential in description of the energy of the system.

2. exam question suggestions

- Which method would you use to solve a large molecule, HF or DFT and why?
- How do exchange and correlation enter the Kohn-Sham equations and what is the meaning of both parts?
- Formulate the rungs of the Jacob's Ladder and give a short description for each rung.
- What is the second Hohenberg-Kohn theorem? Is this theorem a trivial consequence of the first theorem?
- What is the exchange and correlation needed in order to make calculations within DFT?
- What is the main principle of Density Functional Theory (DFT), and how does it differ from traditional wavefunction-based quantum mechanical methods?
- What is the benefit of rewriting the schrodinger equations into the KS equations, and in this fromalism what information is contained in the exchange correlation function?
- What exactly is correlation exchange energy? What are the steps of the Jacobs ladder?
- What do the 'X' and 'C' in XC-function mean? Explain what they represent.
- What is the meaning of exchange-correlation functional in the Kohn-Sham equation?
- How we differentiate Hartee Fork and DFT
- As in the HF vs DFT section which merhod would you use for a specific molecule and why?
- Explain the first Hohenberg-Kohn theorem in your own words
- What is the difference between the correlation energy and exchange energy
- How would you determine the pseudo-potential to be used? If a nodeless orbital contributes to the electron density outside the muffin tin sphere?
- Formulate the first and second HK theorems with your own words
- Explain the role of the exchange potential - how does it differ from classical systems, and how it differs from correlation energy.