

student summaries and exam question suggestions

Density Functional Theory (part 2)

*These pages contain student summaries for the module **Density Functional Theory (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

- **The two Hohenberg-Kohn theorems and why they 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-Plane 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
- consequences 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

- **As in the HF vs DFT section which method 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.