
Excercise Sheet 2

In the next tutorial, we will calculate XAS (x-ray absorption spectroscopy) spectra of a real material using the software "Quanty". Please go through the following exercises for preparation. The tutorial will take place in room REC/B113 at the 17th of may.

Excercise 1: Quanty

"Quanty" is a script language which allows the user to formulate and solve quantum mechanical many body problems. It was written by Maurits Haverkort and can be used free of charge.

Have a look at the Quanty Homepage www.quanty.org.

To get a first impression, go through the tutorials which give the basic ideas of Quanty. They are located at

www.quanty.org/documentation/tutorials/introduction_to_quanty/start.

The tutorials are useful also without installing the software as they always show the input file and the corresponding output. Don't go too much into the details of the code.

Excercise 2 (optional): Play around

If you want, you can try your first own steps with Quanty.

For this register on the homepage www.quanty.org, download Quanty and install it on your computer (see www.quanty.org/documentation/install).

Another option is to go to one of the computer pools (REC/B113, REC/C117) and use the pre-installed Quanty there. To get access to the pools, you need to bring your e-meal card to Mr. Brose in room REC/C116. He will register it such that you can use it to open the doors. The standard ZIH-login is valid for the PCs in these rooms.

Usage of Quanty:

- write your code to a text file e.g. "test.lua"
- open a terminal and change to the directory where you saved the file
- type: `Quanty test.lua`

Exercise 3: XAS on NiO

The nickel ion in the NiO compound has $3d^8$ configuration. This means, there are 8 electrons in the 3d sub-shell, while the lower lying shells are completely filled and therefore not explicitly mentioned. The L-edges in the XAS spectrum are produced by the following process: a photon is absorbed by the nickel ion and thereby one $2p$ core electron is excited to a $3d$ state. What is the configuration of the final state?