Computational Physics Course

Learn to use software packages

Aim of this course

There are a number of software packages prepared for condensed matter physicists, chemists, and material scientists. Those packages have advanced greatly, and are now important tools for researchers as well as learners. In this course, I will provide basic theory behind and let you learn some of the packages.

In 2017, this course (A2 term) starts at 15 November and ends at 10 January, thus consisting of seven days.
Please bring your laptop PC if available.

Lectures

1. First day

Students are requested to install quantum espresso into their PC. The first day is spent in installation. Visit the page A and follow the instruction. I recommend students to install at home and attend the course with the installed PC. We will spend some time with fixing possible problems.

I expect that some of you will not be ready for that. Then, I will just explain the installation and subsequently introduce the modern theory of DFT, which is the main topic of the second day. Note that this is important to understand a frontier of the electronic structure theory.

2. Second day

We begin by learning mostly density functional theory (DFT). I just brief the basics because you have already learned in the previous course and I just focus on a modern aspect, which consists of the adiabatic switching and the fluctuation dissipation theory. If we have time, we will briefly learn the combination of the many-body perturbation theory and DFT.

3. Third day

The computational science lecture should be accompanied by practice of simulation. In this recognition we learn how to use Quantum Espresso, which is one of the most popular free-software. I will probably ask you to draw a band structure of silicon, which is the most elementary step .

4. Fourth day

We will try to understand the band, calculated using the plane wave basis set, in terms of the atomic orbitals. This can be done using the most localized Wannier orbital technology. We will do a calculation of graphene.

5. Fifth day

We will learn the modern theory of polarization, which is one of the most important progress of the electronic structure theory made in 1990s. The theory is based on the most localized Wannier orbital and the density functional perturbation. With those, we can successfully understand the polarization of a crystalline solid.

6. Sixth day

We will simulate the polarization of ferroelectric materials.

7. Seventh day

This is the final lecture. I will provide you with supplemental lecture about DFT, and accept questions about this lecture and reports.

Reports

I will require three reports regarding computer simulation of materials. Details will be shown in the lecture. The evaluation of this A2 term will be done based on the submitted reports, which will be combined with the evaluation made in the A1 term.

Having learned DFT, let us move to learning program packages. We begin by learning Quantum Espresso

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