

CHEM-E4115 - Computational Chemistry I, 27.02.2023-28.04.2023

The course consists of

- 1) Lectures
 - 2) Computer class exercises
 - 3) Independent assignments (6)
- Grading: 0-5 where 0=fail and 5=excellent

Grading is based on the total number of points (max 100 points). The computer class exercises give a maximum of 20 points (0-2 points for each computer class exercise). The 6 independent assignments give a maximum of 80 points and are divided so that the first half of the course (lectured by Kari Laasonen) corresponds to 3 assignments and the second half of the course (lectured by Maria Sammalkorpi) corresponds to 3 assignments. Each set of 3 assignments gives a maximum of 20+10+10=40 points. Each lecturer has one more comprehensive (essay type) assignment and two smaller assignments, which require practical usage of the course learning topics.

Default way of completing the course is to do the course as above. If you want fully DFT or fully soft and biobased materials modelling focus, discuss with lecturer. In that case, you participate only the part matching your choice (2.5 cr). The other 2.5 cr comes from in depth material coverage, project assignment, and associated report in either DFT or molecular modelling.

No points are given for lecture attendance and being present in the computer class exercises is not required for the computer class exercise points (the exercises can be completed independently). However, participation in the lectures and the exercises makes completing the exercises and assignments easier.

Tips:

- Avoid leaving the assignments to the last weekend.
- For both course sections, the 20p assignment (the essay) is the recommended starting point for doing the assignments. Completing the essay first makes the smaller assignments easier.
- Please note that successful completion of the essay requires studying the course material comprehensively (avoid approaches that involve for example reading isolated paragraphs or searching for the key words).

Assignment deadlines:

Assignment 1 (1st essay): **Monday April 3rd, 2023**

Assignments 2-3 (2 smaller assignments): **Thursday April 13th, 2023**

Assignment 4 (2nd essay): **Thursday May 4th, 2023**

Assignments 5-6 (2 smaller assignments): **Tuesday May 9th, 2023**

If completing the course fully focusing on DFT modelling, there is a teacher hour by Kari Laasonen Monday 27th March at 12:15 in B202b. The 2.5 cr project assignment is introduced. Hand-in deadline for it is Tuesday 28th April, 2023.

If completing the course fully focusing on soft and biobased materials modelling, there is a teacher hour by Maria Sammalkorpi Thursday 13th April at 13:15 in B202b. The 2.5 cr project assignment is introduced. Hand-in deadline for it is Tuesday 16th May, 2023.

The completed assignments are submitted for grading in their folder in MyCourses.

Questions:

1st-3rd assignment & DFT part: Kari.Laasonen@aalto.fi

4th-6th assignment & molecular modelling part: Maria.Sammalkorpi@aalto.fi