

CHEM-E4115 - Computational Chemistry I, 28.02.2022-28.04.2022

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.

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 4th, 2022**

Assignments 2-3 (2 smaller assignments): **Wednesday April 20th, 2022**

Assignment 4 (2nd essay): **Thursday May 5th, 2022**

Assignments 5-6 (2 smaller assignments): **Tuesday May 10th, 2022**

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

Questions:

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

4th-6th assignment: Maria.Sammalkorpi@aalto.fi