

## CHEM-E4115 - Computational Chemistry I, 27.02.2023-28.04.2023

### Course outline

Lectures and exercises			Location	Topic	Teacher
27/02/2022	Monday	10:15-12:00	B202b	Atomic total energy, optimization, transition states	Kari Laasonen
02/03/2022	Thursday	13:15-15:00	B202b	Hartree-Fock equations and basis set	Kari Laasonen
03/03/2022	Friday	12:15-14:00	B018	Computer class exercise	Kari Laasonen
06/03/2022	Monday	10:15-12:00	B202b	Correlation and DFT	Kari Laasonen
09/03/2022	Thursday	13:15-15:00	B202b	Bulk systems, k-points, electronic structure	Kari Laasonen
10/03/2022	Friday	12:15-14:00	B018	Computer class exercise	Kari Laasonen
13/03/2022	Monday	10:15-12:00	B202b	Bulk systems continue, surfaces	Kari Laasonen
16/03/2022	Thursday	13:15-15:00	B202b	DFT calculations of surfaces	Kari Laasonen
17/03/2022	Friday	12:15-14:00	B018	Computer class exercise	Kari Laasonen
20/03/2022	Monday	10:15-12:00	B202b	Molecules on surfaces	Kari Laasonen
21/03/2022	Tuesday	10:15-12:00	B018	Computer class exercise	Kari Laasonen
23/03/2022	Thursday	13:15-15:00	B202b	Surfaces reaction	Kari Laasonen
24/03/2022	Friday	12:15-14:00	B018	Computer class exercise	Kari Laasonen
27/03/2022	Monday	10:15-12:00	B202b	Introduction to classical modelling: potential energy surfaces, description of interactions by force-fields	Maria Sammalkorpi
28/03/2022	Tuesday	10:15-12:00	B018	Computer class exercise: Intro to biomolecular MD	Maria Sammalkorpi
30/03/2022	Thursday	14:15-16:00	B202b	Molecular dynamics in practice 1	Maria Sammalkorpi
31/03/2022	Friday	12:15-14:00	B018	Computer class exercise: MD-2	Maria Sammalkorpi
03/04/2022	Monday	10:15-12:00	B202b	Molecular dynamics: controlling the sampling ensembles in simulations (thermostats, barostats etc.)	Maria Sammalkorpi
04/04/2022	Tuesday	10:15-12:00	B018	Computer class exercise: MD-3	Maria Sammalkorpi
05/04/2022	Wednesday	12:15-14:00	B202b	Advanced molecular dynamics approaches	Maria Sammalkorpi
06/04/2022	Thursday			No class because of Easter	
07/04/2022	Friday			No class because of Easter	
10/04/2022	Monday			No class because of Easter	
13/04/2022	Thursday	13:15-15:00	B202b	Teacher hour for those doing the course fully on molecular modelling	Maria Sammalkorpi
17/04/2022	Monday			No class because exam week	
20/04/2022	Thursday			No class because exam week	
21/04/2022	Friday			No class because exam week	
24/04/2022	Monday	10:15-13:00	B202b	Introduction to Monte Carlo methods in molecular modelling, Metropolis Monte Carlo	Maria Sammalkorpi
25/04/2022	Tuesday	10:15-12:00	B018	Computer class exercise: Monte Carlo 1	Maria Sammalkorpi
27/04/2022	Thursday	13:15-16:00	B202b	Monte Carlo methods, continuation; A brief outlook on different simulational methodology (coarse-grained, DPD, continuum, phase-field), General wrap-up	Maria Sammalkorpi
28/04/2022	Friday	12:15-14:00	B018	Computer class exercise: Monte Carlo 2	Maria Sammalkorpi

**NOTE: The following teacher hours only, if doing the course fully on DFT modelling or molecular modelling**

27/03/2022	Monday	12:15-14:00	B202b	Teacher hour for those doing the course fully on molecular modelling DFT	Kari Laasonen
13/04/2022	Thursday	13:15-15:00	B202b	Teacher hour for those doing the course fully on molecular modelling	Maria Sammalkorpi