CHEM-E4115 - Computational Chemistry I, 01.03.2021-29.04.2021
Course outline

	Lectures and exersizes		Topic	Teacher
01/03/2021	Monday	12:15-14:00	Atomic total energy, optimization, transition states	Kari Laasonen
04/03/2021	Thursday	13:15-15:00	Hartree-Fock equations and basis set	Kari Laasonen
05/03/2021	Friday	12:15-14:00	Computer class exercise	Kari Laasonen
08/03/2021	Monday	12:15-14:00	Correlation and DFT	Kari Laasonen
11/03/2021	Thursday	13:15-15:00	Bulk systems, k-points,electronic structure	Kari Laasonen
12/03/2021	Friday	12:15-14:00	Computer class exercise	Kari Laasonen
15/03/2021	Monday	12:15-14:00	Bulk systems continue, surfaces	Kari Laasonen
18/03/2021	Thursday	13:15-15:00	DFT calculations of surfaces	Kari Laasonen
19/03/2021	Friday	12:15-14:00	Computer class exercise	Kari Laasonen
22/03/2021	Monday	12:15-14:00	Molecules on surfaces	Kari Laasonen
23/03/2021	Tuesday	12:15-14:00	Computer class exercise	Kari Laasonen
25/03/2021	Thursday	13:15-15:00	Surfaces reaction	Kari Laasonen
26/03/2021	Friday	12:15-14:00	Computer class exercise	Kari Laasonen
29/03/2021	Monday	12:15-14:00	Introduction to classical modelling: potential energy surfaces, description of interactions by force-fields	Maria Sammalkorpi
30/03/2021	Tuesday	12:15-14:00	Computer class exercise: Intro to biomolecular MD	Maria Sammalkorpi
01/04/2021	Thursday	13:15-15:00	Molecular dynamics in practice 1	Maria Sammalkorpi
06/04/2021	Tuesday	12:15-14:00	Molecular dynamics: controlling the sampling ensembles in simulations (thermostats,	Maria Sammalkorpi
07/04/2021	Wednesday	12:15-14:00	Computer class exercise: MD-2	Maria Sammalkorpi
08/04/2021	Thursday	13:15-15:00	Advanced molecular dynamics approaches	Maria Sammalkorpi
09/04/2021	Friday	12:15-14:00	Computer class exercise: MD-3	Maria Sammalkorpi
13/04/2021	Monday		No class because exam week	
15/04/2021	Thursday		No class because exam week	
16/04/2021	Friday		No class because exam week	
19/04/2021	Monday	12:15-14:00	Advanced molecular dynamics approaches	Maria Sammalkorpi
22/04/2021	Thursday	13:15-15:00	Introduction to Monte Carlo methods in molecular modelling, Metropolis Monte Carlo	Maria Sammalkorpi
23/04/2021	Friday	12:15-14:00	Computer class exercise: Monte Carlo 1	Maria Sammalkorpi
26/04/2021	Monday	12:15-14:00	Monte Carlo methods, continuation	Maria Sammalkorpi
27/04/2021	Tuesday	12:15-14:00	Computer class exercise: Monte Carlo 2	Maria Sammalkorpi
29/04/2021	Thursday	13:15-15:00	A brief outlook on different simulational methodology (coarse-grained, DPD, continuum, phase-field), General wrap-up	Maria Sammalkorpi