CHEM-E4115 - Computational Chemistry I, 28.02.2022-28.04.2022
Course outline

	Lectures and exersizes		Location	Topic	Teacher
28/02/2022	Monday	10:15-12:00	Ke4	Atomic total energy, optimization, transition states	Kari Laasonen
03/03/2022	Thursday	13:15-15:00	Ke3	Hartree-Fock equations and basis set	Kari Laasonen
04/03/2022	Friday	12:15-14:00	B018	Computer class exercise	Kari Laasonen
07/03/2022	Monday	10:15-12:00	Ke3	Correlation and DFT	Kari Laasonen
10/03/2022	Thursday	13:15-15:00	Ke3	Bulk systems, k-points,electronic structure	Kari Laasonen
11/03/2022	Friday	12:15-14:00	B018	Computer class exercise	Kari Laasonen
14/03/2022	Monday	10:15-12:00	B202b	Bulk systems continue, surfaces	Kari Laasonen
17/03/2022	Thursday	13:15-15:00	B202b	DFT calculations of surfaces	Kari Laasonen
18/03/2022	Friday	12:15-14:00	B018	Computer class exercise	Kari Laasonen
21/03/2022	Monday	10:15-12:00	B202b	Molecules on surfaces	Kari Laasonen
22/03/2022	Tuesday	12:15-14:00	B018	Computer class exercise	Kari Laasonen
24/03/2022	Thursday	13:15-15:00	B202b	Surfaces reaction	Kari Laasonen
25/03/2022	Friday	12:15-14:00	B018	Computer class exercise	Kari Laasonen
28/03/2022	Monday	10:15-12:00	B202b	Introduction to classical modelling: potential energy surfaces, description of interactions by force-fields	Maria Sammalkorpi
29/03/2022	Tuesday	12:15-14:00	B018	Computer class exercise: Intro to biomolecular MD	Maria Sammalkorpi
31/03/2022	Thursday	13:15-15:00	B202b	Molecular dynamics in practice 1	Maria Sammalkorpi
04/04/2022	Monday	10:15-12:00	B202b	Molecular dynamics: controlling the sampling ensembles in simulations (thermostats, barostats etc.)	Maria Sammalkorpi
05/04/2022	Tuesday	12:15-14:00	B018	Computer class exercise: MD-2	Maria Sammalkorpi
07/04/2022	Thursday	13:15-15:00	B202b	Advanced molecular dynamics approaches	Maria Sammalkorpi
08/04/2022	Friday	12:15-14:00	B018	Computer class exercise: MD-3	Maria Sammalkorpi
11/04/2022	Monday			No class because exam week	
14/04/2022	Thursday			No class because exam week	
15/04/2022	Friday			No class because exam week	
19/04/2022	Tuesday	10:15-12:00	B202b	Advanced molecular dynamics approaches	Maria Sammalkorpi
21/04/2022	Thursday	13:15-15:00	B202b	Introduction to Monte Carlo methods in molecular modelling, Metropolis Monte Carlo	Maria Sammalkorpi
22/04/2022	Friday	12:15-14:00	B018	Computer class exercise: Monte Carlo 1	Maria Sammalkorpi
25/04/2022	Monday	10:15-12:00	B202b	Monte Carlo methods, continuation	Maria Sammalkorpi
26/04/2022	Tuesday	12:15-14:00	B018	Computer class exercise: Monte Carlo 2	Maria Sammalkorpi
28/04/2022	Thursday	13:15-15:00	B202b	A brief outlook on different simulational methodology (coarse-grained, DPD, continuum, phase-field), General wrap-up	Maria Sammalkorpi