CHEM-E4115 - Computational Chemistry I, 26.02.2024-29.04.2024

Course outline

	Lectures and excersizes		Topic	Teacher
26/02/2024	Monday	10:15-12:00	Atomic total energy, optimization, transition states	Kari Laasonen
29/02/2024	Thursday	13:15-15:00	Hartree-Fock equations and basis set	Kari Laasonen
01/03/2024	Friday	12:15-14:00	Computer class exercise	Kari Laasonen
04/03/2024	Monday	10:15-12:00	Correlation and DFT	Kari Laasonen
07/03/2024	Thursday	13:15-15:00	Bulk systems, k-points,electronic structure	Kari Laasonen
08/03/2024	Friday	12:15-14:00	Computer class exercise	Kari Laasonen
11/03/2024	Monday	10:15-12:00	Bulk systems continue, surfaces	Kari Laasonen
14/03/2024	Thursday	13:15-15:00	DFT calculations of surfaces	Kari Laasonen
15/03/2024	Friday	12:15-14:00	Computer class exercise	Kari Laasonen
18/03/2024	Monday	10:15-12:00	Molecules on surfaces	Kari Laasonen
19/03/2024	Tuesday	10:15-12:00	Computer class exercise	Kari Laasonen
21/03/2024	Thursday	13:15-15:00	surfaces reaction	Kari Laasonen
22/03/2024	Friday	12:15-14:00	Computer class exercise	Kari Laasonen
25/03/2024	Monday	10:15-12:00	Introduction to classical modelling: potential energy surfaces, description of interactions by force-fields	Maria Sammalkorpi
			No class because of spring break	
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04/04/2024	Thursday	13:15-15:00	Molecular dynamics in practice 1	Maria Sammalkorpi
05/04/2024	Friday	13:15-15:00	Computer class exercise: Intro to biomolecular MD	Maria Sammalkorpi
08/04/2024	Monday	10:15-12:00	Molecular dynamics: controlling the sampling ensembles in simulations (thermostats, barostats etc.)	Maria Sammalkorpi
09/04/2024	Tuesday	10:15-12:00	Computer class exercise: MD-2	Maria Sammalkorpi
11/04/2024	Thursday	13:15-15:00	Advanced molecular dynamics approaches	Maria Sammalkorpi
12/04/2024	Friday	13:15-15:00	Computer class exercise: MD-3	Maria Sammalkorpi
15/04/2024	Monday		No class because exam week	
18/04/2024	Thursday		No class because exam week	
19/04/2024	Friday		No class because exam week	
22/04/2024	Monday	10:15-12:00	Introduction to Monte Carlo methods in molecular modelling, Metropolis Monte Carlo	Maria Sammalkorpi
23/04/2024	Tuesday	10:15-12:00	Computer class exercise: Monte Carlo 1	Maria Sammalkorpi
25/04/2024	Thursday	13:15-15:00	Monte Carlo methods, continuation	Maria Sammalkorpi
26/04/2024	Friday	13:15-15:00	Computer class exercise: Monte Carlo 2	Maria Sammalkorpi
29/04/2024	Monday	10:15-12:00 Time was originally wrongly 12:15->	A brief outlook on different simulational methodology (coarse-grained, DPD, continuum, phase-field), General wrap-up	Maria Sammalkorpi