Chemical modelling (KZ7002)

5/12 2024 - 17/1 2025

Teacher:
Alexander Lyubartsev (alexander.lyubartsev@mmk.su.se) Lectures

Assistent:
Maksim Posysoev (maksim.posysoev@mmk.su.se) Exercises and project

Week	Time	Monday	Tuesday	Wednesday	Thursday	Friday
49 2/12-6/12	9.15-12.00 13.00-16.00				**L1** -	**L2**
50 9/12 – 13/12	9.15-12.00 13.00-16.00	**L3** **E1**	**L4** **E1***	**L5** -	**L6** -	**Lab / project**
51 16/12 –20/12	9.15-12.00 13.00-16.00	**L7** -	**L8** -	**Lab / project**	**Lab / project**	**L9** -
52,1 23/12-6/01	9.15-12.00 13.00-16.00				**JULLOV**	
2 6/1–10/1	9.15-12.00 13.00-16.00		**L10** **E2**	**Lab / project**	**Lab / project**	**Lab / project**
13/1 –17/1	9.15-12.00 13.00-16.00	**Lab / project**	**L11** -	**project** **presentations**	**L12** -	**Exam**

* - additional time if needed

Place:
Lectures and exercises: KÖL, TBA

Computer laborations: in the form of project (at MMK)

Exam: KÖL

Literature:

All the course content will be covered by the lecture notes. As additional reading the following book is recommended:
A.R.Leach: Molecular modeling. Principles and applications (2nd edition).

Lectures content:

Lecture	Content	Chapters from the book *
L1	Introduction to Chemical Modelling	(1)
L2	Quantum mechanics: fundamentals	(2)
L3	Quantum chemistry and electron structure calculations (Hartree-Fock, correlation methods, basis sets)	2
L4	Density functional theory	3
L5	Statistical thermodynamics. Statistical ensembles.	**
L6	Method Monte Carlo	8
L7	Molecular interactions. Molecular mechanics. Force field.	4,5
L8	Molecular dynamics	6,7
L9	Mesoscale simulations (Coarse-grained models; Langevine and Brownian dynamics; DPD)	-
L10	Computation of thermodynamic properties (free energies, biased simulations, metadynamics)	8,11
L11	Applications in biochemistry and material science	(10,12)
L12	Repetition: questions and answers	-

*: in parenthesis: not fully covered: use lectures material
**: use Chapter 11 from P. Atkins, J. de Paula, R. Friedman "Physical Chemistry: Quanta, Matter and Change"

Problem solving exercises

E1 Exercises: quantum mechanics and quantum chemistry
E2 Exercises: statistical thermodynamics and simulations

Computer laborations / project

MMK room C513 (eventually KÖL), possibility for remote access @home

13 Dec: Introduction to the project / choice of the system / planing . Introduction to work with Linux OS, terminals, remote connection, etc
18 Dec - 13 Jan: Execution of the project
15 Jan: Presentations of the project