

Chemical modeling (KZ7002)

30/11 2017 - 12/1 2018

Teachers:

Alexander Lyubartsev (A) alexander.lyubartsev@mmk.su.se

Erik Brandt (E) erik.brandt@mmk.su.se

Assistent:

Bojan Vujic (B) bojan.vujic@mmk.su.se

Week	Time	Monday	Tuesday	Wednesday	Thursday	Friday
49 27/11-1/12	9.15-12.00 13.00-16.00				L1 -	L2 -
50 4/12 – 8/12	9.15-12.00 13.00-16.00	L3 -	L4 -	L5 -	Lab 1	Nobel Lectures
51 11/12 –15/12	9.15-12.00 13.00-16.00	Lab 2	L6 E1	Lab3	L7 -	L8 -
52 18/12-22/12	9.15-12.00 13.00-16.00	Lab 4	L9 -	Lab 5	L10 E2	Jullov
1 1/1–5/1	9.15-12.00 13.00-16.00	Jullov			Lab 6	L11 -
2 8/1 –12/1	9.15-12.00 13.00-16.00	L12 E3		L13 -		Exam

Place: room K****

Problem solving exercises

E1 Exercises: quantum mechanics and quantum chemistry (B)

E2 Exercises: statistical thermodynamics (B)

E3 Group exercises: modeling methods and applications (A)

Computer laborations:

Computer laborations will take place in room C513 of the Arrhenius laboratory, 9.00 - 16.00

Lab 1. Quantum chemistry: geometry optimization

Lab 2. Reactions and catalysis

Lab 3. DFT in solid state

Lab 4. Molecular dynamics

Lab 5. Mesoscale simulations

Lab 6 Gas sorption in porous materials (Monte Carlo)

Literature:

A.R.Leach: Molecular modeling. Principles and applications.(2nd edition)

Lectures content:

Lecture	Content	Teacher	Chapters from the book *
L1	Introduction to Chemical Modelling. Mathematical repetition.	E	(1)
L2	Quantum mechanics: fundamentals	A	(2)
L3	Quantum chemistry and electron structure calculations (LCAO, Hartree-Fock, correlation methods)	A	2
L4	Density functional theory	A	3
L5	Statistical thermodynamics. Statistical ensembles.	A	**
L6	Metod Monte Carlo	A	8
L7	Molecular interactions. Molecular mechanics. Force field	E	4,5
L8	Molecular dynamics	E	6,7
L9	Mesoscale simulations (Coarse-grained models; Langevine and Brownian dynamics; DPD)	E	-
L10	Computation of thermodynamic properties (free energies, biased simulations, metadynamics)	E	8,11
L11	Applications in biochemistry and material science	E	(10,12)
L12	Hardware and software issues, data formats, visualization; postanalysis	E	-
L13	Repetition: questions and answers	A,E	-

*: 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"