Chemical modeling (KZ7002)

6/12 2018 - 18/1 2019

Teachers:
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Week	Time	Monday	Tuesday	Wednesday	Thursday	Friday
49 3/12-7/12	9.15-12.00 13.00-16.00				**L1** -	**L2** -
50 10/12 – 14/12	9.15-12.00 13.00-16.00	**L3** **E1**	**L4** -	**Lab 1**	**Lab 2**	**L5** -
51 17/12 –21/12	9.15-12.00 13.00-16.00	**L6** -	**Lab 3**	**L7** -	**L8** -	**Lab 4**
1 31/12-4/1	9.15-12.00 13.00-16.00	**J U L L O V**				
2 7/1–11/1	9.15-12.00 13.00-16.00	**L9** -	**Lab 5**	**L10** **E2**	**L11** -	**Lab 6**
3 14/1 –18/1	9.15-12.00 13.00-16.00	**L12** **E3**		**L13** -		**Exam**

Place:
Lectures and exercises: KÖL. Kxxx see TimeEdit schedule at www.kemi.su.se

Problem solving exercises

E1 Exercises: quantum mechanics and quantum chemistry (M)
E2 Exercises: statistical thermodynamics and simulations (M)
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 Monte Carlo (sorption)

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.	A	(1)
L2	Quantum mechanics: fundamentals	A	(2)
L3	Quantum chemistry and electron structure calculations (Hartree-Fock, correlation methods, basis sets)	A	2
L4	Density functional theory	A	3
L5	Statistical thermodynamics. Statistical ensembles.	A	**
L6	Method 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"