

KEMM48/NAKE09 (2021) – Statistical Thermodynamics and Molecular Simulation

Division of Theoretical Chemistry, Lund University

Schedule

This schedule is preliminary and may be subject to changes.

Date	Time		Room	Chapter	Lecturer
Mon 18/1	09:00–10:00	Roll call	KC:A/Zoom	Only master students	
Mon 18/1	10:15–12:00	Lecture 1	Zoom	1-3	JF
Thu 21/1	10:15–12:00	Lecture 2	Zoom	4,6	JF
- " -	13:15–15:00	Exercise 1	Zoom		JF/MT
Mon 25/1	10:15–12:00	Lecture 3	Zoom	7,20, B-Williams (notes)	MT
Thu 28/1	13:15–15:00	Lecture 4	Zoom	15,17	MT
- " -	13:15–15:00	Exercise 2	Zoom		JF/MT
Mon 1/2	10:15–12:00	Lecture 5	Zoom	Simulations (notes)	ML
Thu 4/2	10:15–12:00	Lecture 6	Zoom	Coarse-graining (notes)	ML
- " -	13:00–15:00	Research@Teokem	Zoom	Presentation of the lab+mingle	All
Mon 8/2	08:30–12:30	Lab exercise 1	Zoom	Mandatory (all)	MT
Thu 11/2	10:15–12:00	Lab lecture 2	Zoom	Molecular Dynamics	A,H,S
Mon 15/2	08:30–12:30	Lab exercise 2	Zoom	Mandatory (all)	A,H,S
Thu 18/2	10:15–12:00	Lecture 7	Zoom	18, electrical double layer	MT
- " -	13:15–15:00	Exercise 3	Zoom		JF/MT
Fri 19/2	23:59	Hand-in Lab 1	First draft	via email (comments by 21/2)	
Mon 22/2	10:15–12:00	Lecture 8	Zoom	gvdW (notes)	JF
Thu 25/2	08:15–12:00	Lab exercise 3	Zoom	Mandatory (Group A)	H
- " -	13:15–17:00	Lab exercise 3	Zoom	Mandatory (Group B)	H
Mon 1/3	10:15–12:00	Lecture 9	Zoom	13, 21.1-2, polymers (notes)	JF
Thu 4/3	10:15–12:00	Exercise 4	Zoom		JF/MT
Fri 5/3	23:59	Hand-in Lab 2+3	First drafts	via email (comments by 21/2)	
Mon 8/3	10:15–12:00	Exercise 5	Zoom		JF/MT
Thu 11/3	10:15–12:00	Lecture 10	Zoom	repetition, examples	MT
Thu 18/3	08:00–13:00	Exam	Zoom		
Tue 23/3	23:59	Hand-in Labs 1-3	Final reports	via email	
Fri 23/4	08:00–13:00	Re-exam	Zoom?		
Fri 27/8	08:00–13:00	Re-exam 2	Zoom?		

Book

Roland Kjellander “Statistical Mechanics of Liquids and Solutions: Intermolecular Forces, Structure and Surface Interactions Volume’ I’, CRC Press, ISBN 978-1482244014

Frenkel Daan and Smit Berend, “Understanding Molecular Simulation (Second Edition)“, Academic Press, ISBN 978-0-12-267351-1

(freely available online thorough a Lund University license on:
<http://www.sciencedirect.com/science/book/9780122673511>).

These books are complemented by hand-out material.

Lecturers

Jan Forsman (JF), Mikael Lund (ML), and Martin Trulsson (MT) at Theoretical Chemistry.

Tutorials

The tutorials will be supervised by JF and MT at Theoretical Chemistry.

Laborations

The lab practicals will be supervised by Vidar Aspelin (A), Stefan Hervö-Hansen (H) and Samuel Stenberg (S) at Theoretical Chemistry.

Evaluation

Written exam.

Contact

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