

KEMM38/NAKE09 (2019) – 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 25/3	09:30–10:00	Roll call	B	Only master students	
Mon 1/4	10:15–12:00	Lecture 1	K	1-3	JF
- " -	13:15–15:00	Lecture 2	K	4,6	JF
Tue 2/4	10:15–12:00	Lecture 3	S	7,20, B-Williams (notes)	MT
- " -	13:15–15:00	Exercise 1	S		ZY
Wed 3/4	10:15–12:00	Lecture 4	L	15,17	MT
- " -	13:15–15:00	Exercise 2	L		ZY
Thu 4/4	10:15–12:00	Lecture 5	L	18, electrical double layer	MT
- " -	13:15–15:00	Exercise 3	M		ZY
Fri 5/4	10:15–12:00	Lecture 6	K	Simulations (notes)	ML
- " -	13:15–15:00	Lecture 7	K	Coarse-graining (notes)	ML
Tue 23/4	10:15–12:00	Lab lecture I	L/Teokem	Molecular Dynamics	A,H,S
- " -	13:15–17:00	Lab exercise I	L/Teokem		A,H,S
Wed 24/4	10:15–12:00	Lecture 8	L	gvdW (notes)	JF
- " -	13:15–15:00	Exercise 4	L		ZY
Thu 25/4	10:15–12:00	Lecture 9	L	13, 21.1-2, polymers (notes)	JF
- " -	13:15–15:00	Exercise 5	L		ZY
- " -	15:00–17:00	Research@Teokem	Teokem	Presentation of the lab+mingle	All
Fri 26/4	10:15–12:00	Lecture 10	L	repetition, examples	MT
- " -	13:15–15:00	Exercise 6	L		ZY
Mon 13/5	23:59	Hand-in Lab I	First draft	via email (comments by 17/5)	
Wed 15/5	08:00–13:00	Exam	H,I		
Thu 16/5	08:15–12:00	Lab exercise II	Teokem	Group A	JD
- " -	13:15–17:00	Lab exercise II	Teokem	Group B	JD
		(PhD course)		(Mon 20/5–Thu 23/5)	
Fri 24/5	23:59	Hand-in Labs I	Final report	via email	
Mon 27/5	23:59	Hand-in Lab II	First draft	via email (comments by 31/5)	
Fri 7/6	23:59	Hand-in Labs II	Final report	via email	

Book

Terrell L. Hill, “An Introduction to Statistical Thermodynamics”, Dover Publications, ISBN 0-486-65242-4

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 Zakiyeh Yousefian (ZY) at Theoretical Chemistry.

Laborations

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

Evaluation

Written exam.

Contact

Martin Trulsson – martin.trulsson@teokem.lu.se