"Advanced Course in Modern Molecular Modelling"

A graduate course - given together by Theoretical Chemistry Dept at KTH and Physical Chemistry division at Stockholm University.

http://www.theochem.kth.se/courses/ACM3.html

Part 3: Macroscopic Concept - Statistical thermodynamics (8 ETSC credits)
Part 4: Molecular Modelling - Learning to Fly (8 ETSC credits)

The two parts will go in parallel, two lectures per day, part 3 on Tuesdays & Fridays, and part 4 on Thursdays

time: 10.00-12.00 and 13.00-15.00

Part 3: Macroscopic Concept - Statistical thermodynamics (8 ETSC credits)

1/9 (Tue)	L1 Statistical thermodynamics: Boltzmann distribution (S) L2 Thermodynamics 1 (A)
4/9 (Fri)	L3 Statistical thermodynamics: Canonical ensemble (S) L4 Thermodynamics 2 (A)
8/9 (Tue)	L5 Grand-canonical and other ensembles (S) Lab: Simulated Boltzmann (S)
11/9 (Fri)	L6 Stat.therm: Ideal systems 1 (translational + rotational partition function) (S) P1: Problem solving exercises (S)
15/9 (Tue)	L7: Stat. therm: Ideal systems 2 (vibrational p.f, normal modes) (S) L8 Applications in spectroscopy (A)
18/9 (Fri)	L9: Statistical thermodynamics: Lattice systems (S) L10: Kinetics 1 (A)
22/9 (Tue)	L11: Quantum statistical thermodynamics (S) L12 Kinetics 2 (A)
25/9 (Fri)	L13: Virial expansion, Theories of liquid state (S) P2: Problem solving exercises (A)
29/9 (Tue)	L14: Electrolytes and polyelectrolytes (S) P3: Problem solving exercises (S)
6/10 (Tue)	Examination

Literature: *D.A.McQuarrie, Statistical Mechanics, University Science Books, 2000.*

Part 4: Molecular Modelling - Learning to Fly (8 ETSC credits)

(Thuesdays)

10/9 10:00 **L1** Simulation methods & Molecular Mechanics (A)
13:00 **L2** Method Monte Carlo (S)

17/9 10:00 **L3** Molecular Dynamics background (A)
13:00 **L4** Ewald summation, Free energy and generalised ensembles (S)

24/9 10:00 **L5** Molecular Dynamics techniques & applications (Aatto)
13:00 **L6** MDynaMix tutorial + choice of projects (Sasha)

1/10 10:00 **L7** Car-Parrinello MD (Sasha)
13:00 **L8** Mesoscale modelling (Aatto)

8/10 10:00 **L9** Multiscale modelling (Aatto)
13:00 **L10** Quantum simulations (Sasha)

12/10 - 11/11 Project work

Thu 12/11 10:00 **Presentation of projects**

Aatto – Aatto Laaksonen (aatto@physc.su.se) Phone: 162372
Sasha – Alexander Lyubartsev (sasha@physc.su.se) Phone: 161193

Literature: Andrew R. Leach, Molecular Modelling – Principles and Applications (II Edition)
Lecture notes and other course materials will be given.

Contact either Aatto or Sasha if you are interested!