

“Advanced Course in Modern Molecular Modelling (ACM3)”

Part 4, 2007-2008, September/October 2008

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#part4>

Part 4: Molecular Modelling (8 ETSC credits)

Lectures are given in lecture room K205 (except 25/9 in K418) at the undergraduate education building (Kemiska övningslaboratoriet – KÖL, enter just next to Frescatihallen), Stockholm University

time: 10.00-12.00 and 13.00-15.00

Fri 19/9 10:00 L1 Simulation methods & Molecular Mechanics (Aatto)

Fri 19/9 13:00 L2 Method Monte Carlo (Sasha)

Wed 24/9 10:00 L3 Molecular Dynamics background (Aatto)

Wed 24/9 13:00 L4 Ewald summation, Free energy and generalised ensembles (Sasha)

Thu 25/9 10:00 L5 Molecular Dynamics techniques & applications (Aatto)

Thu 25/9 13:00 L6 MDynaMix tutorial + choice of projects (Sasha)

Wed 1/10 10:00 L7 Mesoscale modelling (Aatto)

Wed 1/10 13:00 L8 Car-Parrinello MD (Sasha)

Thu 2/10 10:00 L9 Multiscale modelling (Aatto)

Thu 2/10 13:00 L10 Quantum simulations (Sasha)

3/10 - 21/10 Project work

Thu 23/10 10:00 **Presentation of projects**

Aatto – Aatto Laaksonen (aatto-at-physc.su.se) Phone: 162372

Sasha – Alexander Lyubartsev (sasha-at-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!