

General course information

Registration for the IVC-SEP advanced course is only possible by e-mail to Anne Louise Biede, alb@kt.dtu.dk

Please include a billing address in your registration e-mail!

Further information: Ioannis G. Economou, e-mail: ie@kt.dtu.dk

Registration deadline: 30 April 2008

Prices:	Before 1 April	After 1 April
Industrial participant	€ 2,200	€ 2,400
IVC consortium member	€ 1,100	€ 1,200
Non-DTU PhD student	€ 250	€ 300
DTU PhD student	free	free
Academic	€ 1,100	€ 1,200

Payment procedure:

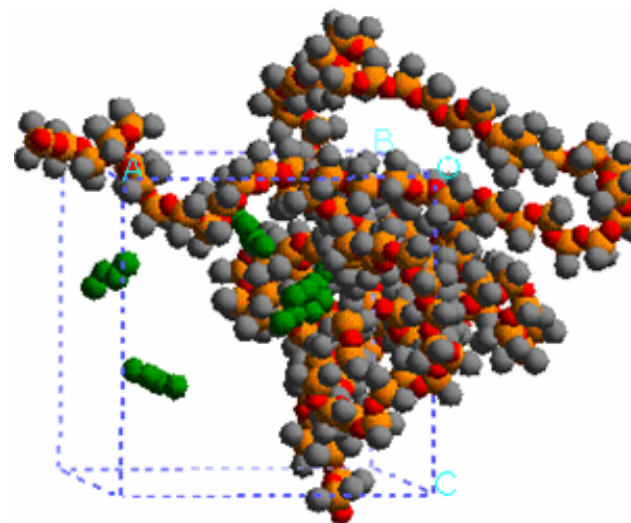
Registered participants will receive an invoice that should be paid before 10 May 2008. Since there is a maximum in the number of participants, an early registration is recommended.

Advanced Course on Molecular Simulation of Complex Chemical Systems with Emphasis to Practical Applications

2 – 13 June 2008

by

Ioannis G. Economou



www.ivc-sep.kt.dtu.dk

Course description

The course will provide the participants with a knowledge of fundamental principles of statistical mechanics and thermodynamics, of how to link microscopic phenomena with macroscopic properties and of how to model complex chemical systems.

The course is of relevance to researchers involved in molecular modeling, molecular thermodynamics, polymer physics and physical chemistry of fluids. People involved in process and / or advanced material design will benefit from it.

Fundamentals: Introduction to statistical mechanics, statistical ensembles, intermolecular potentials, Monte Carlo simulation, Molecular Dynamics simulation, Molecular Mechanics.

Advanced simulation techniques: Efficient calculation of phase equilibria (Gibbs ensemble and extended ensemble simulations), calculation of chemical potential, elementary Monte Carlo moves for chain molecules, polymers, biomolecules etc.

Applications: Phase equilibria of pure fluids and mixtures; Gas solubility in polymers; Molecular design of gas separation membranes.

Prerequisites: Undergraduate courses in Physical Chemistry and / or Chemical Thermodynamics, working knowledge of Fortran

The Centre for Phase Equilibria and Separation Processes at the Department of Chemical Engineering, DTU, was founded in 1980 by the late Prof. A. Fredenslund and in 1988 it was named an Engineering Research Center (IVC) by the Danish Research Council. From the very beginning, molecular thermodynamics has been the essential subject of the centre. The course will give the students insight into the fundamentals of statistical mechanics and molecular thermodynamics, scientific programming and molecular design computational tools.

Curriculum: Two weeks of lectures, classroom problems and computer exercises

Exam: During the following two weeks (from 16 to 27 June) the participants will work on a major exam problem and write a report. This work can be carried out elsewhere. Participants are welcomed to work on a major problem of their own choice. The problem should be suggested to teacher in the first three days of course.

Additional information:

Maximum number of participants: 20

The course credits are 7.5 ECTS points

Course material:

D.A. McQuarrie, *Statistical Mechanics*, Harper and Row, New York, 1976.

D. Frenkel and B. Smit, *Understanding Molecular Simulation*, Academic Press, 1996.

Teacher's extended power point slides, notes and papers (will be posted on course website)