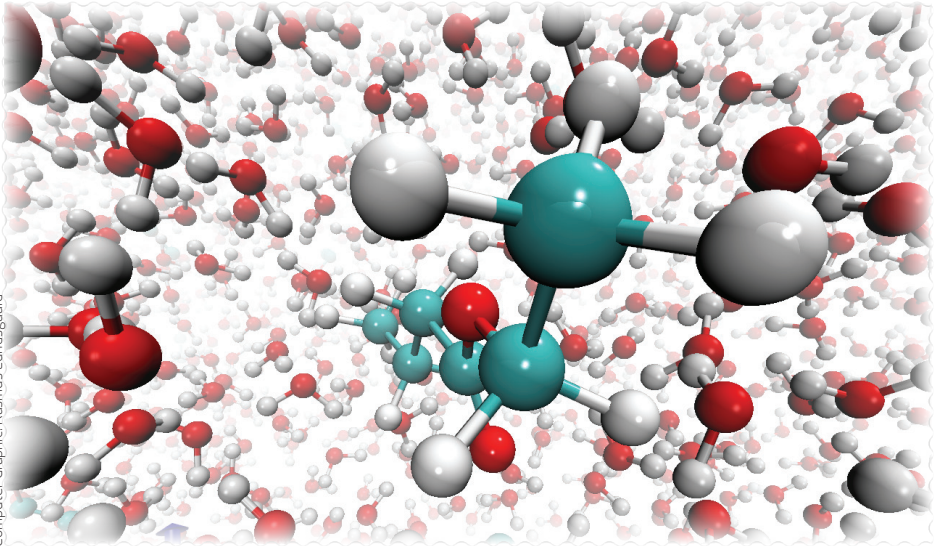
Advanced Course on Molecular Simulation of Complex Chemical Systems with Emphasis to Practical Applications



Computer Graphic: Rasmus Lundsgaard

28 June - 9 July 2010

by

Prof. Vlasis G. Mavrantzas

Univ. of Patras & FORTH-ICE/HT, GREECE

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 Mechanic, Dissipative Particle Dynamics, Iterative Boltzmann Inversion method for the calculation of effective potentials

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:

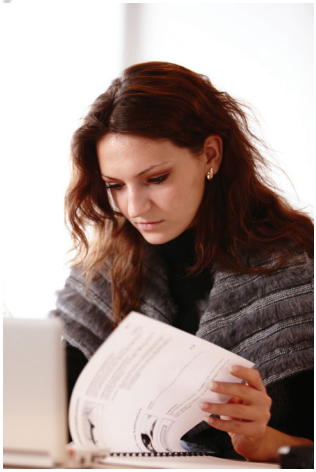
Phase equilibria of pure fluids and mixtures, Gas solubility in polymers, Molecular design of gas separation membranes, Water transport through carbon nanotubes, Gas transport in polymer electrolyte membranes

Prerequisites:

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

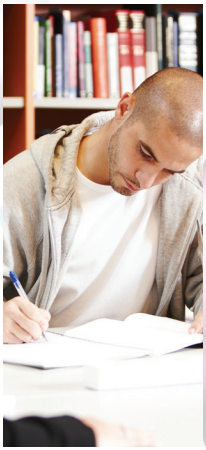
Curriculum: Two weeks of lectures, classroom problems and computer exercises

Exam: During the two weeks following the course (from 28 June – 9 July 2010) 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:

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

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

3. D.N.Theodorou and V.G. Mavrantzas, Multiscale Modeling of Polymers, Oxford Univ. Press, in preparation, 2010

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

General course information

Registration for the CERE advanced course:
https://conferences.dtu.dk

Further information: Vlasis Mavrantzas, email vlasis@chemeng.upatras.gr or Georgios Kontogeorgis, e-mail: gk@kt.dtu.dk

Registration deadline: 1 April 2010

Prices:	Before 1 April	After 1 April
Industrial participant	€ 2,400	€ 2,500
CERE consortium member	€ 1,300	€ 1,400
PhD student	€ 250	€ 300
Academic	€ 1,300	€ 1,400

Payment procedure:

Payment and registration - use the webpage https://conferences.dtu.dk.

Since there is a maximum in the number of participants, an early registration is recommended.

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
Technical University of Denmark
Søltoft Plads
Building 229

Layout: Christian Carlsson Photo: Colourbox.com