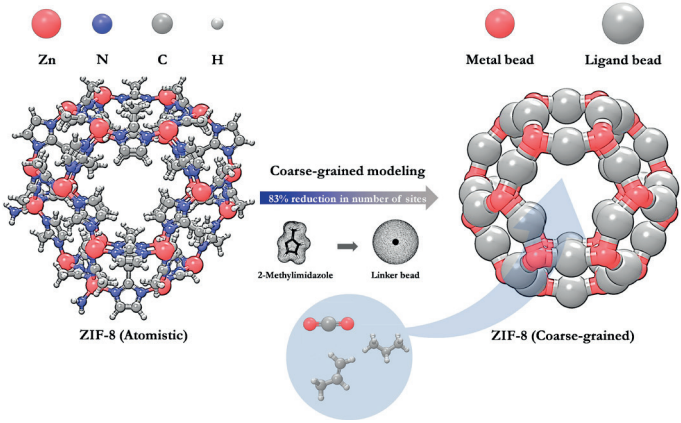
Advanced Course
on
Molecular simulation of fluids: Fundamentals and industrial applications



Monday 3 - Friday 21 March 2025

CERE
Department of Chemical & Biochemical Engineering
Technical University of Denmark

Course description

Duration of the course:

Two weeks of lectures and computer problems (24 hrs lectures + 24 hrs problem sessions):

a. 4 days a week (Monday – Thursday): 9 am – 12 noon (lectures),
b. 1 – 4 pm problem sessions.

In the third week, students will work on a team project.

Course description:
Molecular simulation has evolved as a very powerful tool for accurate calculation of structure and properties of complex chemical systems. Properties include thermodynamic, mechanical, rheological, electrical and many others. The unprecedented increase of computing power at affordable price has made molecular simulation very popular in chemical and process engineering research and industrial practice.

Course content:
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 in single or mixed phases.

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

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:
Prediction of thermophysical properties (i.e., density, compressibility, fugacity, etc.); Phase equilibria of pure fluids and mixtures; Gas solubility in polymers; Electrolyte solutions; Molecular design of gas separation membranes; Modeling of mixed matrix membranes; Metal organic frameworks; Ionic liquids; Hydrate phase equilibria.

Prerequisites:
The course is intended for advanced Master students and PhD students in Chemical Engineering, Materials Science or Chemistry. Post-docs or industry professionals are welcome. Good knowledge of Physical Chemistry and / or Chemical Thermodynamics, and of Numerical Methods is needed.

The course will be of relevance to researchers involved in molecular modeling, molecular thermodynamics, material design and physical chemistry of fluids. People involved in process design will benefit from it.

Point (ECTS) 7,5

Course format:
The course will consist of lectures and hands-on computer exercises. The students will be asked to work on a team project and submit a report at the end of the course.
Access to the high performance computing system of DTU is needed. Students will work on LAMMPS or GROMACS.

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).

Course instructor:
The course instructor will be Dr. Ioannis G. Economou, Otto Mønsted Visiting Professor at Technical University of Denmark. He has more than 30 years of experience in molecular thermodynamics and molecular simulation of complex fluids.

General course information

Venue:
Department of Chemical & Biochemical Engineering, DTU, Lyngby, Denmark
The course will be offered in hybrid format. Online attendance will be possible.

Information about course site and links will be provided in advance to the course participants.

Registration: www.cere.dtu.dk/education/phd-courses

Further information: Olivia Perederic (oper@kt.dtu.dk)

Professor Ioannis G. Economou. Photo: Christian Ove Carlsson

Registration deadline: February 21, 2025
Payment deadline February 21, 2025

Prices:

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

Since there is a maximum of about 30 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