Molecular Thermodynamics (CENG0027)

Description

Aims:
With the present emphasis on nano and bio technologies, molecular level descriptions and understandings offered by statistical thermodynamics are of increasing interest and importance.

The aim of this module is to describe what statistical thermodynamics is, and to emphasize how chemical engineers can use it to advance practical applications.

One goal is to demonstrate how molecular level approximations are applied to understand the physical world, how macroscopic thermodynamic models engineers use derive from such approximations, and the importance of remembering the approximations assumed while developing the models.

The students will become familiar with molecular-level computer simulations.

Learning Outcomes:
On successfully completing the module, the students will:

- relate concepts taught in classical thermodynamics to intermolecular interactions;
- recognize the basics of statistical thermodynamics;
- learn the fundamentals of commonly used molecular simulation techniques, such as Monte Carlo and molecular dynamics;
- employ molecular simulation techniques to calculate macroscopic properties from intermolecular forces;
- relate molecular-level understanding of matter to a number of modern practical applications

Synopsis:
This course studies the theories for describing and predicting the phase equilibria of systems of interest to the modern chemical engineer. It starts with a description of classical thermodynamics concepts, focusing on how such concepts depend on our understanding of intermolecular
interactions. The discussion will focus on how statistical thermodynamics techniques allow us to predict macroscopic properties from the knowledge of intermolecular interactions and other molecular properties. The statistical mechanics framework will be used to introduce the modern tools of Monte Carlo and molecular dynamics simulations. A demonstration of how the results of molecular simulations can be used to enrich the molecular theories of matter will follow. Finally, there will be a discussion on how statistical thermodynamic concepts are useful for advancing practical applications.

Examples will include, but will not be limited to, self-assembling structures, materials and processes for separations, and strategies for energy storage.
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Key information
Year: 2019/20
Credit value: 15 (150 study hours)
Delivery: UGM L7, Campus-based
Reading List: View on UCL website
Tutor: Prof Alberto Striolo
Term: Term 1
Timetable: View on UCL website

Assessment
- Open-book examination (main exam period): 40%
- Coursework: 40%
- Coursework: 20%

Find out more
For more information about the department, programmes, relevant open days and to browse other modules, visit ucl.ac.uk

Disclaimer: All information correct as of August 2019. Please note that aspects of the module may be subject to change. UCL will make best efforts to inform applicants of major changes.
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