

# **Project work – thermodynamic assessment**

## **Practical information**

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**CHEM-E6115: Thermodynamics of modeling and simulation**

# Aims of the practical work

- Become aware of computational thermodynamics and software
- Understand the basic philosophy of doing a thermodynamic assessment
- Experience the basic work flow in thermodynamic assessment by doing an assessment of a simple binary eutectic system and writing a report about it

# Project work

- Perform assessment in groups of two people
- Every group assesses a binary eutectic system using the Factsage software -> stable phases considered only
- Written report of the work is required
- Systems to be freely chosen from given list
- You can learn from the published articles for the well assessed systems of your assignment

# Additional information

- Deadline of the report is by the end of May
- The report should be maximum 20 pages, containing:
  - (i) detailed literature survey, evaluation and selection, of experimental data
  - (ii) model description and model selection and
  - (iii) Optimized thermodynamic parameters
  - (iv) Final results of the plots you can make.
- Also, the OPT-file, and the CDB and SLN- data files should be provided

# Software

- The program FactSage can be installed on Aalto computers with access to the Factsage server.
- Factsage is available on common computer in F-wing, 4<sup>th</sup> floor.
  - I will check if I can get access for everyone to the server
  - I will assist in installing the Factsage program
  - It requires a working Aalto-VPN
- Factsage Edu can be installed on your personal computers, can be used to do calculations, but not optimizations. Limited to 3 elements
- [http://www.factsage.com/FactSageEdu\\_Info.htm](http://www.factsage.com/FactSageEdu_Info.htm)
- <http://www.factsage.com>

# Upcoming actions

- Selection of groups
  - Organize yourselves into groups of two and inform me by Friday, April 1.
  - Option: I will arrange groups randomly after that.
- Installation of Factsage software
  - Installation of Factsage Edu can be done by yourselves on your personal computer
  - For optimization, full version is needed.
    - Inform me if you want it installed on your computer and reserve time with me for installation.
    - Option is to use the installation at Aalto

# Upcoming actions

- Select chemical system to be studied – I will provide several examples by end of the week.
  - Metallic, ceramic, organic
  - In case you are interested in specific chemical systems, let me know and I will try to make a suitable suggestion
- Preparation of database and demonstration of optimization, time to be decided
- Make literature survey of all available experimental thermodynamic and phase equilibrium data for your system, potentially also published assessment works
- Short progress meetings

# Date for project seminar

- Mid May
  - Short 10-15 minute presentations on the progress of the assessment
- Final version of project work can be handed in until May 31