# CHEM-E6115 Thermodynamics of modeling and simulation (5 cr)

Examination Responsible teacher: prof. Daniel Lindberg

April 13, 2022

Answer both questions, and utilize handouts, course material, as well as the references given below (should be accessible with Aalto VPN), or other sources you find from scientific literature. It is not mandatory to refer to all sources in you answer, but if additional sources are used, please indicate the source. The essay must be uploaded at the latest on Wednesday April 27, at 16:00. If further information is needed, contact me at daniel.k.lindberg@aalto.fi

1. Describe **one** experimental method for measuring phase equilibria and thermodynamic properties (4 points) from the following topics:
   1. Differential scanning calorimetry (DSC)
   2. Solution calorimetry
   3. Drop calorimetry
   4. Equilibration-Quenching method
   5. EMF method

The description should include the following:

- Main working principle of method

- Chemical system/materials that are suitable for the method

- Suitable conditions for the method (e.g. temperature range, pressure, sample size)

- Advantages/disadvantages compared to other similar methods

1. Describe the general features of **one** thermodynamic solution model and describe the type of chemical system they are suitable for (4 points)
   1. Quasichemical model
   2. Associate model
   3. Sublattice model
   4. Regular solution model

The description should include the following:

- Main feature of the model

- Chemical system/materials that are suitable for the method

- Advantages/disadvantages compared to other similar models

References

[New Developments in the Calorimetry of High-Temperature Materials - ScienceDirect](https://www.sciencedirect.com/science/article/pii/S2095809918307367?via%3Dihub)

[Progress and New Directions in Calorimetry: A 2014 Perspective - Navrotsky - 2014 - Journal of the American Ceramic Society - Wiley Online Library](https://ceramics.onlinelibrary.wiley.com/doi/10.1111/jace.13278)

[Methods for Phase Diagram Determination | ScienceDirect](https://www.sciencedirect.com/book/9780080446295/methods-for-phase-diagram-determination)

[Phase Diagrams and Thermodynamic Modeling of Solutions | ScienceDirect](https://www.sciencedirect.com/book/9780128014943/phase-diagrams-and-thermodynamic-modeling-of-solutions)

[The need for reliable data in computational thermodynamics (nih.gov)](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7558216/pdf/nihms-1616309.pdf)

[Overview: The emf method as a source of experimental thermodynamic data - ScienceDirect](https://www.sciencedirect.com/science/article/pii/S0364591610000386?via%3Dihub)