LECTURES AND PRATICAL TRAINING

GENERAL INFORMATION

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This school is organized for the third time. The previous two successful schools (2014 and 2015) were organized close to Paris. In 2017, the SATA school will be held in the Presqu'Ile de Giens in the south of France.

Important note:

All students have to bring a laptop for use during the school. All teaching will use the Thermo-Calc software.

The demo version of Thermo-Calc can be downloaded from:

http://www.thermocalc.com/productsservices/software/test-drive-demo/

Organizers

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Information

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Registration

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Location

Presqu'Ile de Giens, France

hotel Belambra "les Criques":
http://www.belambra.fr/club-presqu-ile-de-giens-les-criques/

SATA

School for Advanced Thermodynamic Assessments

Presqu'Ile de Giens, France 3-7 July, 2017

The aim of the school is to provide an advanced course on thermodynamic modelling using the Calphad method. A central part of the school will be the practical assessment of model parameters of multi-component systems for the development of thermodynamic databases. Such databases are a fundamental part of the materials genome initiative and for the Integration of Computational Materials.
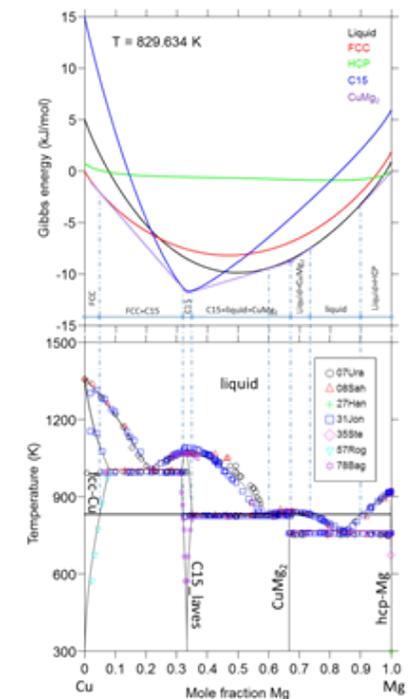
Develop models for the Gibbs energy of individual phases (top) in order to calculate phase diagrams (bottom) representing experimental data.

Scope

The central theme of the teaching is computational thermodynamics and the school will teach practical assessment of multicomponent systems using thermodynamic models. The importance and use of different kinds of theoretical and experimental data will be explained and how theoretical calculations can be combined with experimental data by thermodynamic models and integrated in multi-component databases applicable to modem materials.
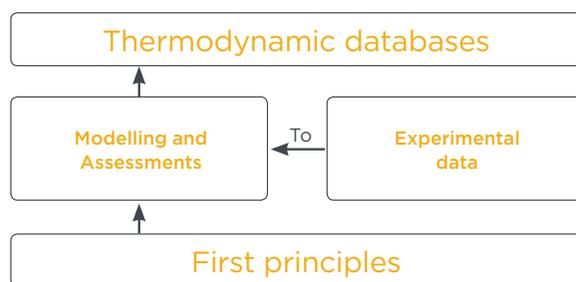
Who should participate ?

PhD students, post-docs and scientists,

➔ working with assessment of thermodynamic systems and interested to gain a better understanding of modelling and how to handle the assessment software,

➔ wishing to enhance their comprehension as to how atomistic simulations can be applied for establishing multi-components phase equilibria and diagrams,

➔ interested in learning how to model defects, interstitial solutions, chemical and magnetic ordering,

➔ wishing to become familiar with the coupling between thermodynamics, phase diagrams and microstructures,

➔ interested in integrating thermodynamic databases in simulations of phase transformations.

Monday : Calphad and experimental data

• Welcome and presentations of teachers and students
• Calphad basic techniques and models
• Experimental techniques, calorimetry
• Experimental techniques, phase diagram
• Software Session 1: Basic examples on individual laptop

Tuesday: Calphad and theoretical data

• Models for ordering
• Experimental techniques, activity measurements
• First Principles methods 1
• Creating setup and experimental data files
• Software Session 2: Assessment practice

Wednesday: Thermodynamic assessments

• First principles methods 2
• Special modelling for ionic systems
• Software Session 3: Assessment practice
• General questions and anwers
• **Afternoon: Free time**

Thursday: Validation of assessment

• Presentation of results by the students
• Software session 4: Assessment practice
• Stable and metastable extrapolations
• Software session 5: Assessment practice
• Documentation and reporting

Friday: Integration and feedback

• Presentation of results by students
• Integration of assessments in multi-component data-bases and software
• Evaluation and feedback to teachers and software developers by all

Summary

More than half of time at the school is devoted to practical assessment of real systems by the students with assistance by experts. The Cu-Mg system has been selected as a case study as it has many important modelling features. However, the students are encouraged to bring the systems they are currently working on for discussions.

A week is too short to perform a complete assessment of

any system but the students will have a chance to understand how the available software tools can be used in particular cases.

Registration deadline: 26 May 2017

LANGUAGE:
English

FEE:
€ 1600

INCLUDES:
Accommodation, meals, local transport.

LOCATION:
Hotel Belambra, Presqu'Ile de Giens, France.

Transfers will be available from the train station and airport in Toulon.