

## Computational Thermodynamics and Kinetics Seminar

Welcome to the Thermo-Calc Software User Group Meeting 2024 in Leoben, Austria.

### PROGRAM:

**Thursday February 29, 2024**

- 12:00 – 13:00**     *Registration*
- 13:00 – 14:00**     *Lunch*
- 14:00 – 14.15**     **Welcome and Introduction**  
*Andre Schneider, Thermo-Calc Software AB, and Jiehua Li, Chair of Casting Research, Montanuniversität Leoben*
- 14:15 – 14:40**     **News from Thermo-Calc, Overview of recent developments, Outlook to the future**  
*Andre Schneider, Thermo-Calc Software AB*
- 14:40 – 15:05**     **Process Metallurgy Simulations for the Transition to Hydrogen-Based Iron- and Steelmaking**  
*Alisson Kwiatkowski da Silva, Nicholas Grundy, Ralf Rettig, Lina Kjellqvist, Thermo-Calc Software AB*
- 15:05 – 15:30**     **High-throughput calculations with TC-Python for alloy optimisation**  
*Ulrich Klotz, fem Research Institute, Schwäbisch Gmünd, Germany*
- 15:30 – 15:55**     **Ru-containing hardmetals: experimental studies and thermodynamic calculations**  
*Raquel de Oro Calderon, Lena Maria Dorner, Wolf-Dieter Schubert, Ralph Useldinger, TU Wien, Vienna, Austria*
- 15:55 – 16:30**     *Coffee break*
- 16:30 – 16:55**     **CALPHAD dataset development for the systems Nb/Ta-Al-O**  
*Julian Gebauer, Peter Franke, Hans Jürgen Seifert, Karlsruhe Institute of Technology, IAM-AWP, Germany*
- 16:55 – 17:20**     **TCP phases, can it be that a model based on binary interactions, respecting crystallography and using DFT, works also for multicomponent extrapolations?**  
*Suzana G. Fries, Ruhr University Bochum, Germany*
- 17:20 – 17:45**     **Modeling of phase equilibria and diffusion in Sn-Ag-Cu solder systems**  
*Roman Čička, Marian Drienovsky, Tereza Machajdikova, Institute of Materials Science, Slovak University of Technology, Trnava, Slovakia*
- 17:45 – 18:10**     **Die Steel Design for Additive Manufacturing**  
*Florian Hengsbach, Julius Bürger, Anatolii Andreiev, Krista Biggs, Jörg Fischer-Bühner, Jörg Lindner, Kay-Peter-Hoyer, Mirko Schaper, Greg Olson, Paderborn University & Massachusetts Institute of Technology, Germany & USA*
- 18:10 – 18:35**     **Composition screening by combining TC Python and MICRESS: Solidification microstructures of Al recycling alloys as an example**  
*Markus Apel, Access e.V., Aachen, Germany*
- 19:30 – late**     *Social gathering and dinner at Arkadenhof Gaststätte Schwarzer Adler*  
Address: Hauptplatz 11, 8700 Leoben

**Friday March 01, 2024**

- 08:30 – 08:55**    **Combination of computer thermodynamic simulation tools and experiments to understand the early stage precipitation of sigma phase in high alloyed duplex steels**  
*Aurélie Jacob, TU Wien, Vienna, Austria*
- 08:55 – 09:20**    **How Thermo-Calc Software incorporates in modelling Kirkendall porosity in compositionally graded Ni-based superalloys**  
*Ahmadreza Riyahi Khorasgani, Ingo Steinbach, Julia Kundin, ICAMS, Ruhr Universität Bochum, Germany*
- 09:20 – 09:45**    **Thermodynamic and kinetic modelling of precipitation processes in Inconel 800HT alloy during the exploitation**  
*Hanna Purzyńska, Roman Kuziak, Łukasz Poloczek, Łukasiewicz Research Network – Upper Silesian Institute of Technology, Gliwice, Poland*
- 09:45 – 10:10**    **Modeling the bainite start temperature with CALPHAD by integration of ab-initio data**  
*Tobias Spitaler, Bernd Schuscha, Lorenz Romaner, Montanuniversität Leoben, Department Materials Science, Leoben, Austria*
- 10:10 – 10:35**    **ICME for sustainable and reliable manufacturing**  
*David Linder, John Aristeidakis, Ida Berglund, QuesTek Europe AB, Solna, Sweden*
- 10:35 – 11:05**    ***Coffee break***
- 11:05 – 11:30**    **Incorporating vacancies into 3rd generation CALPHAD descriptions: A case study for the Al-Ni system**  
*Alexander Walnsch, Andreas Leineweber, Mario J. Kriegel, TU Bergakademie Freiberg, Institute of Materials Science, Germany*
- 11:30 – 11:55**    **The CALPHAD method and its predictive capabilities - case study for the Al-Cu-Si system**  
*Ales Kroupa, Ondrej Zobac, Klaus W. Richter, Academy of Science of the Czech Republic, Institute of Physics of Materials, Brno, Czech Republic*
- 11:55 – 12:20**    **The Thermo-Calc Additive Manufacturing Module: An integrated CALPHAD-based FEM tool**  
*Andre Schneider, Andreas Markström, Amer Malik, Quang Minh Do, Johan Jeppsson, Thermo-Calc Software AB*
- 12:20 – 12:45**    **Designing high performance Al-based composites with Thermo-Calc**  
*Jiehua Li, Chair of Casting Research, Department of Metallurgy, Montanuniversität Leoben*
- 12:45 – 13:00**    **Closing remarks / Wrap up**
- 13:00 – 14:00**    ***Lunch***
- 14:00 – 15:30**    **Lab Tour of the Chair of Casting Research**  
*Jiehua Li, MU Leoben - Chair of Casting Research, Department of Metallurgy, Leoben*

**LOCATION:** Seminarraum "D", Chair of Casting Research, Montanuniversität Leoben

