

## Computational Thermodynamics and Kinetics Seminar

Welcome to the Thermo-Calc Software user group meeting Hosted by Royce at the University of Sheffield, at the Sir Robert Hadfield Building on June 11-12, 2024.

### PROGRAM, Day 1, June 11:

- 09.30 – 10.15** *Registration with refreshments*
- 10.15 – 10.30** **Welcome and Introduction**  
*Carl-Magnus Lancelot, Thermo-Calc Software*
- 10.30 – 11.10** **News from Thermo-Calc Software: Thermo-Calc, DICTRA, TC-PRISMA and databases**  
*Carl-Magnus Lancelot, Thermo-Calc Software*
- 11.10 – 11.35** **Design of oxidation resistant Nb-Si alloys aided by computational thermodynamics**  
*Claire Utton, University of Sheffield*
- 11.35 – 12.05** *Short break with snacks and drinks*
- 12.05 – 12.30** **Using DICTRA to simulate external oxidation for steel tubes in high temperature processing applications**  
*Megan Kendall, Swansea University Bay Campus*
- 12.30 – 12.50** **Simulation of solidification and phase formation in the Mg-rich corner of Mg-Ca-Zn alloys**  
*Yanheng Xie, University of Sheffield*
- 12.50 – 13.10** **Assessing the Printability of Steels with Computational Thermodynamics and Machine Learning**  
*Raymond Wong, Imperial College London*
- 13.10 – 14.30** *Lunch in the Turner Museum*
- 14.30 – 14.50** **Optimisation of advanced steel design for fusion energy applications**  
*David Bowden, UK Atomic Energy Agency*
- 14.50 – 15.10** **Design of new boron-strengthened reduced activation ferritic-martensitic steels for fusion**  
*Jack Haley, UK Atomic Energy Agency*
- 15.10 – 15.30** **The Preliminary research of NbTiZr-X (X=Al, Mo, Ta, W, Cr) of RCCAs through Thermo-Calc**  
*Yu-Hsuan Lee, University of Sheffield*
- 15.30 – 16.00** *Short break with snacks and drinks*
- 16.00 – 16.25** **Mean-field model for hydride evolution within Zircalloys**  
*Connor Cladingboel, University of Sheffield*
- 16.25 – 17.00** **Demonstration of Additive Manufacturing module, with the new Keyhole model and printability maps**  
*Magnus Anderson, Thermo-Calc Software*
- 19.30** **Dinner**  
*Location TBA*

For more information about Thermo-Calc, please visit:

[www.thermocalc.com](http://www.thermocalc.com)

# Thermo- Software

## **PROGRAM, Day 2, June 12:**

- 09.00 – 9.30** *Registration with refreshments*
- 9.30 – 9.40** **Day 2 Welcome and Introduction**  
*Carl-Magnus Lancelot, Thermo-Calc Software*
- 9.40 – 10.00** **Designing new ultra-radiopure, high-strength electroformed CuCr alloys, for rare event searches**  
*Dimitra Spathara, University of Birmingham*
- 10.00 – 10.20** **Phase Prediction and Validation of AlSiFeCrCoNi Multi Principal Element Alloys**  
*Thon Thongklom, University of Sheffield*
- 10.20 – 10.40** **Application of Thermo-Calc with machine learning towards the design of carbon reinforced high entropy alloys for metal forming tooling applications**  
*Joshua Berry, University of Sheffield*
- 10.40 – 11.05** **Thermo-Calc calculations of gas turbine engine mineral deposit melting temperatures**  
*Jacob Elms, University of Manchester, Earth and Environmental Sciences*
- 11.05 – 11.30** *Short break with snacks and drinks*
- 11.30 – 11.55** **Ordering regimes in Zirconium Carbides**  
*Theresa Davey, Bangor University, Wales*
- 11.55 – 12.20** **Experimental investigation and thermodynamic modelling of WC-40Fe-20Co-40Ni**  
*Tomas Soria Biurrun, CEIT, Spain*
- 12.20 – 12.45** **Enhancing industrial materials using ICME**  
*Hoda Dini, Questek Europe*
- 12.45 – 13.00** **Closing remarks / Wrap Up**
- 13.00 – 14.30** *Lunch in the Turner Museum*
- 14.30 – 16.00** *Tour of the Royce Centre*

## **REGISTRATION:**

Please send your registration for the seminar via E-Mail before May 25 with your full name and address to: Thermo-Calc Software AB, [info@thermocalc.com](mailto:info@thermocalc.com). Please indicate if any special requirements for food are needed, such as vegetarian or non-dairy.

Seminar fee: 100 GBP per day, waived for presenters.

Dinner fee: 50 GBP

**LOCATION:** Sir Robert Hadfield Building, University of Sheffield

Turner Museum of Glass and Lecture room LT21

<https://www.sheffield.ac.uk/turner-museum/visitor-information>

WELCOME!

*For more information about Thermo-Calc, please visit:*

**[www.thermocalc.com](http://www.thermocalc.com)**