

## 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.

This programme is preliminary, and is likely to be updated before the Seminar.

### 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 – 11.20** **News from Thermo-Calc Software: Thermo-Calc, DICTRA, TC-PRISMA and databases**

*Carl-Magnus Lancelot, Thermo-Calc Software*

**11.20 – 11.50** *Short break with snacks and drinks*

**11.50 – 12.15** **Design of oxidation resistant Nb-Si alloys aided by computational thermodynamics**

*Claire Utton, University of Sheffield*

**12.15 – 12.40** **Ordering regimes in Zirconium Carbides**

*Theresa Davey, Bangor University, Wales*

**12.40 – 13.15** **Simulation of solidification and phase formation in the Mg-rich corner of Mg-Ca-Zn alloys**

*Yanheng Xie, University of Sheffield*

**13.15 – 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** **Title pending**

*Jack Haley, UK Atomic Energy Agency*

**15.10 – 15.40** *Short break with snacks and drinks*

**15.40 – 16.05** **Title pending**

*Connor Cladingboel, University of Sheffield*

**16.05 – 16.30** **Title pending**

*Daniel Cogswell, University of Sheffield*

**16.30 – 17.00** **Demonstration of Additive Manufacturing model, with the new Keyhole model and printability maps**

*Magnus Anderson, Thermo-Calc Software*

**19.30** **Dinner**

*Location TBA*

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# Thermo- Software

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

- 09.00 – 9.30** *Registration with refreshments*
- 9.30 – 9.45** **Day 2 Welcome and Introduction**  
*Carl-Magnus Lancelot, Thermo-Calc Software*
- 9.45 – 10.35** **Demonstration of capabilities of Process Metallurgy Module**  
*Nicholas Grundy, Thermo-Calc Software*
- 10.35 – 11.00** **Thermo-Calc calculations of gas turbine engine mineral deposit melting temperatures**  
*Jacob Elms, University of Manchester, Earth and Environmental Sciences*
- 11.00 – 11.30** *Short break with snacks and drinks*
- 11.30 – 11.55** **Using DICTRA to simulate external oxidation for steel tubes in high temperature processing applications**  
*Megan Kendall, Swansea University Bay Campus*
- 11.55 – 12.20** **Experimental investigation and thermodynamic modelling of WC-40Fe-20Co-40Ni**  
*Tomas Soria Biurrun, CEIT, Spain*
- 12.20 – 12.45** **TBA**  
*Author, Affiliation*
- 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.

This programme is preliminary, and although it seems full, it might be possible to fit one or two extra presenters.

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!

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