



CALPHAD L

50th International Conference on Computer Coupling of Phase Diagrams and Thermochemistry

June 25th – 30th, 2023

Cambridge, MA, USA





Agenda and Abstracts

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*Celebrating the 50th anniversary of the CALPHAD conference
and its homecoming to MIT in memory of Larry Kaufman*

“We believe that substantial progress can be made in a short period of time if we could arrange to work together for one week at one of our facilities to define problems, disband, carry out some individual activities, and meet again for a week at a second facility to compare results and chart future activities.”

— Larry Kaufman and Himo Ansara, 1973

Preface

It is very appropriate that, on its 50th anniversary, the Calphad Conference should return to the city of its origin. From an original attendance of approximately 12 scientists at CALPHAD 1, the attendance now has to be restricted to ensure all can be accommodated at CALPHAD 50! CALPHAD is truly a major success story. It has made, and continues to make, major contributions in the field of materials science, in particular to the development and practical application of materials of many different types. The interest in the ‘Calphad method’ is world-wide, as exemplified by the CALPHAD conferences taking place in cities across the Globe.

The first CALPHAD conference took place when the computer was a very new tool in the laboratory, when there were serious concerns about calculation methods and the suitability of different models being used to link binary and ternary alloy data, not to mention big disagreements on appropriate nomenclature. Such concerns have long since disappeared and the advances since CALPHAD 1 have been very impressive. A glance through the titles of the presentations at CALPHAD 50 provides clear evidence of the enormous scope for calculations resulting from the linking of thermodynamic theory with sophisticated methods for measuring and theoretically deriving the necessary input data.

Philip Spencer

In returning CALPHAD to its MIT Kaufman-Cohen origins, it is appropriate to acknowledge the extraordinary vision of Larry Kaufman in transforming the materials discipline from an engineering science to a scientific engineering, enabled by his conceived infrastructure of fundamental phase-level data we now know as the Materials Genome, and his founding of an international organization to create and maintain it. It is this infrastructure of fundamental data and supporting software that has allowed us for the first time to put to practical use, in a system-specific and quantitative way, the fundamental mechanistic understanding that the science of materials has gleaned over the past century. As a tribute to Kaufman’s vision, this conference will emphasize the historic achievements in CALPHAD-based acceleration of materials design and development that has transformed the materials profession as practiced by leading corporations in aerospace, automotive and consumer electronics sectors, with ever-broadening application across materials classes.

Greg Olson

We are thrilled to witness the tremendous response to the CALPHAD 50, with an impressive turnout of nearly 200 participants representing over 20 countries. The caliber of the abstract submissions has been truly outstanding, making the task of selecting oral and poster presentations an arduous endeavor. We have kept the CALPHAD tradition without introducing parallel session for oral presentations, complemented by an extensive 6-hour poster session. These formats provide an optimal platform for exchanging ideas and forging connections that will shape the future of the CALPHAD research.

Participating in the CALPHAD conference is always an exceptional experience. Researchers, experts, and enthusiasts converge to share their knowledge and expertise under such a positive and amiable ambiance. The spirit of collaboration permeates every aspect of the event, and we are deeply grateful for the trust placed in us by the CALPHAD community to organize this significant gathering for the 50th anniversary. We believe that the conference will not only provide intellectual stimulation but also deliver an enjoyable and rewarding experience for all.

Wei Xiong & Yu Zhong

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CALPHAD L Conference Organizing Committee

Organizers Prof. Yu (Michael) Zhong (Worcester Polytechnic Institute)
 Prof. Wei Xiong (University of Pittsburgh)

Organizing Committee Prof. Gregory B. Olson (Massachusetts Institute of Technology)
 Prof. Raymundo Arróyave (Texas A&M University)
 Prof. Scott McCormack (University of California, Davis)
 Dr. Richard Otis (NASA Jet Propulsion Laboratory)

International Scientific Advisory Committee

Chair: Zi-Kui Liu, USA

Members:

Mark Asta, USA

Claude Bernard, France

Tim Chart, UK

Gabriele Cacciamani, Italy

Yong Du, China

Zhenmin Du, China

Bengt Hallstedt, Germany

Jean-Marc Joubert, France

Ursula Kattner, USA

K.C. Hari Kumar, India

Byeong-Joo Lee, Korea

In-Ho Jung, Korea

Hiroshi Ohtani, Japan

Arthur Pelton, Canada

André Schneider, Germany

Hans Seifert, Germany

Malin Selleby, Sweden

Marcel Sluiter, Netherland

Philip Spencer, USA

Bo Sundman, Sweden

Axel van de Walle, USA

Andy Watson, UK

Ping Wu, Singapore

Sponsors



STIFTELSEN
FÖR TILLÄMPAD
TERMODYNAMIK

THERMFACT



CALPHAD L Conference Agenda Overview (June 25-30, 2023)

Updated on 6/6/2023	Sunday 6/25	Monday 6/26	Tuesday 6/27	Wednesday 6/28	Thursday 6/29	Friday 6/30
Morning		○ Breakfast	○ Breakfast	○ Breakfast	○ Breakfast	○ Breakfast
		Session 1 8:00AM	Session 3 8:00AM	Session 5 8:00AM	Session 6 8:00AM	Session 8 8:00AM
Noon		○ Lunch 12:30PM	○ Lunch 12:30PM	○ Lunch 12:30PM	○ Lunch 12:30PM	○ Box Lunch 12:30PM
Afternoon	○○ Materials Genome Toolkit Workshops, 1-4 PM & Registration 4-8 PM	Session 2 2:00PM	Session 4 2:00PM	Excursion Duck Tour Boarding 2:00 PM (Firm!!!) Group photo MIT Great Dome 5:15pm	Session 7 2:00PM	
	○○ Welcome Reception 6-8 PM (Salon III) Finger-food & drink provided	○ Dinner 6:00PM ○ Poster session (1) 7:00-10:00 PM	○ Dinner 6:00PM ○ Poster session (2) 7:00-10:00 PM	○ Dinner 6:00PM ○ Young Calphadian Night, 7:00-10:00 PM	○○○ Odyssey Dinner Cruise, 6:30 PM Banquet and Award Announcement	

Color code for locations and more information:

- **Boston Marriott Cambridge Hotel** (50 Broadway, Cambridge, MA 02142)
Materials Genome Toolkit Workshops (2nd floor), Registration, and Welcome Reception (Salon III)
- **Wong Auditorium, Tang Center (Campus bldg. No. E51)**
Coffee breaks & Oral presentation sessions
- **The 7th floor of the Samberg Conference Center (Campus bldg. No. E52)**
Meals, Poster sessions, and Young Calphadian Night
- ▨ **Excursion Duck Tour, Boarding start from 2:00 PM on 6/28 Wed (Firm!!!)**
Boarding from Marriott hotel from the side facing the Main Street!
- **Group photo, 5:15pm on 6/28 Wed.**
Please gather in front of the MIT great dome facing the river side and Memorial Drive
- **Odyssey Dinner Cruise, 6:30 PM, 6/29 Thursday**
Bus will be waiting in front of the Marriott Cambridge hotel at 6:00PM

Conference Site and Floor Plans

Boston Marriott Cambridge Hotel (Address: 50 Broadway, Cambridge, MA 02142)



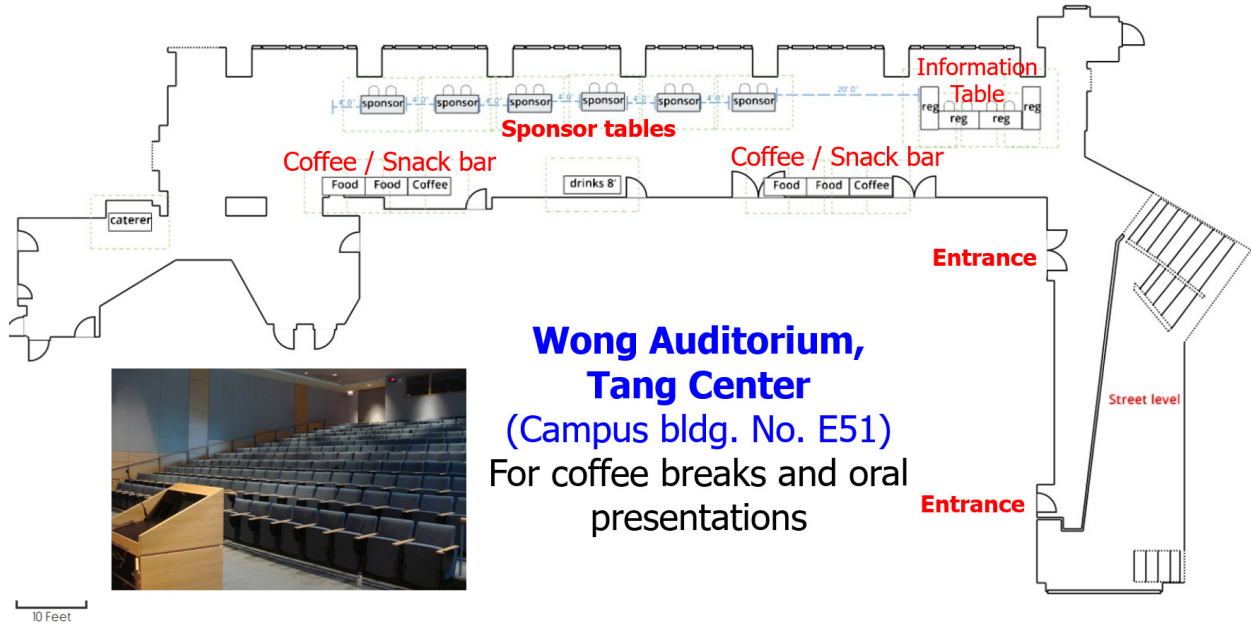
Wong Auditorium, Tang Center (2 Amherst St, Cambridge, MA 02142) MIT

7th floor, Samberg Conference Center (50 Memorial Dr, Cambridge, MA 02142) MIT



About five minutes walking distance between the hotel and conference rooms.

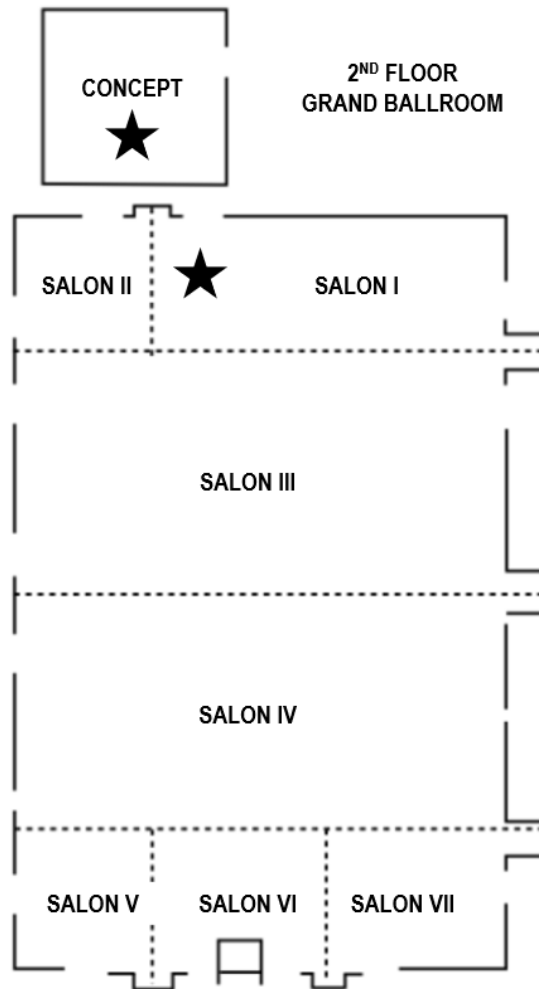
	<p>Materials Genome Toolkit Workshops, registration, and reception will be at the <u>Boston Marriott Cambridge Hotel</u>.</p> <p>Coffee breaks & oral sessions will be at the <u>Wong Auditorium, Tang Center</u> (Campus bldg. No. E51)</p> <p>Meals, Poster sessions, Young Calphadian Night will be on the 7th floor of the <u>Samberg Conference Center</u> (50 Memorial Drive), (bldg. No. E52)</p> <p>The APDIC committee meeting will be held in one of the smaller dining rooms (#6) on the 6th floor of the <u>Samberg Conference Center</u>, 2-5 PM, Friday, June 30</p>
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Boston Marriott Cambridge Hotel

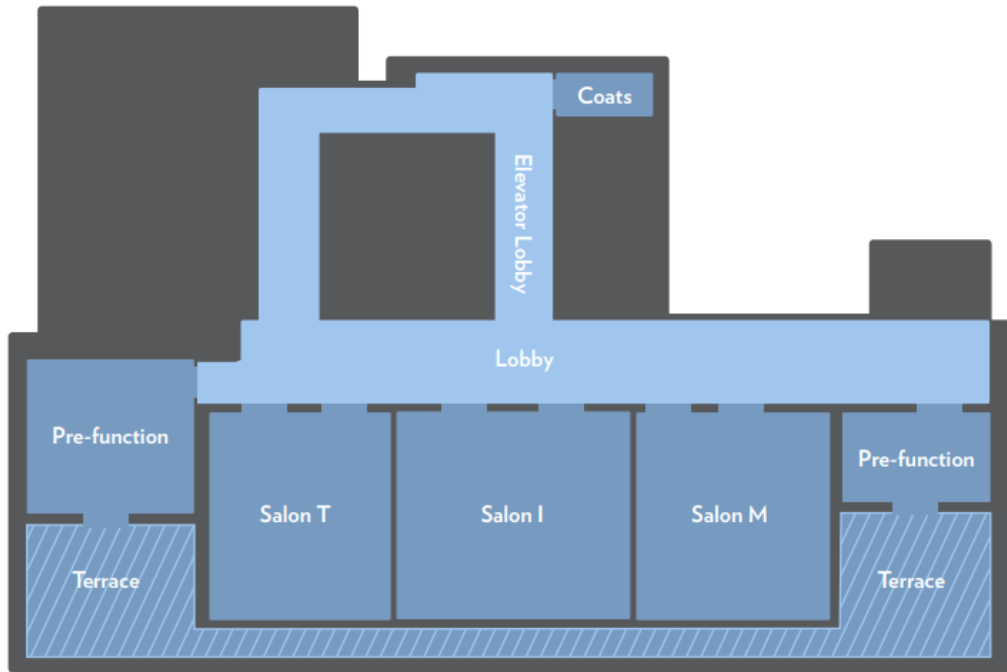
Conference Rooms for Workshop (Concept, Salon I & II), Registration, and Welcome Reception (Salon III)

Rooms are on the 2nd floor. Concept room (stairs or elevator available), and Salon I-II room (located at the top of the escalator from the main lobby)



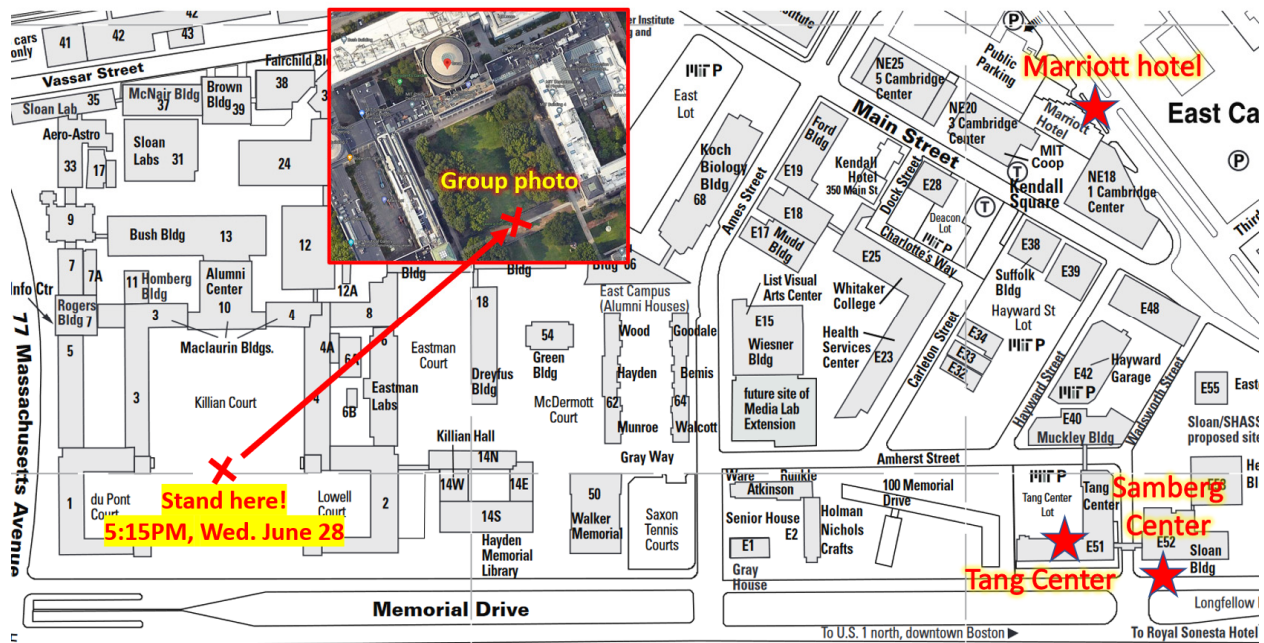
Samberg Conference Center, 7th floor

Meals, Poster Sessions, and Young Calphadian Night will be here.



Group Photo, 5:15pm on 6/28 Wed, Location:

Please gather in front of the MIT Great Dome facing the river side and Memorial Drive. Standing point is marked below (x)



Social Program

Duck Tour, Wednesday, June 28, 2023, Boarding at 2:00 PM (Firm!!!)

Boarding directly outside from the Marriot hotel, but from the side facing Main Street.

Conference registrants and their accompanying guests are invited to join a Duck Tour of Boston aboard a W.W.II style amphibious landing vehicle that travels on land and water. The tour will depart from Kendall Square, which is within walking distance from the conference.



<https://bostonducktours.com/>

Space is limited; tickets must be reserved at the time of registration.

Odyssey Dinner Cruise, Thursday, June 29, 2023.

Boarding starts at 6:30 PM, Cruise from 7:00 – 10:00 PM

Bus will be wait outside of the Boston Marriot Cambridge Hotel at 6:00 PM

All conference registrants and their accompanying guests are cordially invited to join us for an enchanting evening aboard the Odyssey Dinner Cruise on Boston Harbor. Awards will be announced during the cruise dinner. Complimentary transportation to and from the cruise will be provided for your convenience.

<https://www.cityexperiences.com/boston/city-cruises/our-fleet/odyssey-boston/>



CALPHAD Materials Genome Toolkit Workshops

Note: Two workshops will be running in parallel at the Boston Marriott Cambridge Hotel
Coffee will be served for 1-hour between 2-3PM.

Workshop 1: Diffusion Mobility Assessment Best Practices and Developing a CALPHAD Data Infrastructure

Time: 1-4 PM, US Eastern Time, Sunday, June 25, 2023

Location: Concept (2nd floor; stairs or elevator available)

Diffusion Data and Mobility Assessments (Presenter: Carelyn Campbell, NIST)

1:00-1:20 Best Practices for Diffusion Data:

- Review of best practices for acquiring and analyzing diffusion data, including available tools (e.g., pyDiffusion)

1:20-1:45 Best practices for Diffusion Mobility Assessments

- Review of best practices and examples, including available tools (e.g., pyMob,)
- Optimization of mobilities using composition profiles

1:45-2:00 Discussion of best practices and future needs

CALPHAD-based Diffusion Tools

2:00-2:45 CALPHAD-based Diffusion Tools (highlighting how the diffusion data are used)

- CompuTherm Tools, *Presenters: Shuanglin Chen and Chuan Zhang, CompuTherm, LLC (20 minutes)*
- MICRESS, *Presenter: Markus Apel, Access e.V. (20 minutes)*

2:45-3:00 Discussion of CALPHAD-based diffusion tools

CALPHAD Data Infrastructure

3:00-3:15 Democratization of CALPHAD data (*Noah Paulson, ANL*)

3:15-3:30 XML-based TDB formats (*Bo Sundman, OpenCALPHAD, KTH*)

3:30-3:45 Future formats for optimization (POP files) discussion

3:45-4:00 CALPHAD-based benchmark discussion

Workshop 2: Software Tools from Machine Learning to Phase Diagrams

Instructors: Richard Otis, Jet Propulsion Laboratory; Brandon Bocklund, Lawrence Livermore National Laboratory; Adam M. Krajewski, Pennsylvania State University

Time: 1-4 PM, US Eastern Time, Sunday, June 25, 2023

Location: Salons I-II (located at the top of the escalator from the main lobby)

Introduction:

This workshop will give a detailed introduction to computational thermodynamic software based on the CALPHAD method – pycalphad and ESPEI - as well as an introduction to machine learning methods in computational materials science. It will feature hands-on demonstrations in an interactive cloud environment and practical exercises that will enable attendees to perform machine learning calculations, develop CALPHAD databases with quantified uncertainty, and to propagate uncertainty to any thermodynamic calculation. Attendees are encouraged to bring their laptop or computing device to follow along interactively. Tables, power outlets, and WiFi will be provided.

pycalphad

pycalphad is a free and open-source Python library for calculating phase diagrams, designing thermodynamic models, and investigating phase equilibria within the CALPHAD method. It provides routines for reading thermodynamic databases and solving the multi-component, multi-phase Gibbs energy minimization problem. All Gibbs energy and property models in pycalphad are described symbolically allowing the models to be customized or overridden by users at runtime without changing any of the pycalphad source code. Calculation results from pycalphad are returned as multidimensional xarray datasets that make it easy to incorporate pycalphad into any tool or workflow.

ESPEI

The Extensible Self-optimizing Phase Equilibria Infrastructure (ESPEI) package is a tool for thermodynamic database development and uncertainty quantification within the CALPHAD method. It uses pycalphad for the forward calculation of thermodynamic properties to solve the inverse of the parameter evaluation problem. ESPEI uses a two-step method to first parameterize thermodynamic models and then optimize and determine the uncertainty of the parameters using Markov Chain Monte Carlo (MCMC).

pySIPFENN

The Python-toolset for Structure-Informed Prediction of Formation Energy using Neural Networks (pySIPFENN) is an open-source tool designed to assist researchers in predicting the results of time and cost-intensive calculations like first-principles calculations based on the density functional theory (DFT). pySIPFENN provides a streamlined, intuitive interface to perform formation energy predictions on large sets of atomic structures with high accuracy and low computational cost. It plays a crucial role in the rapid, low-cost generation of the protodata that ESPEI can use for thermodynamic database development. The software comes with pre-trained models, with advanced users having the ability to utilize customized models. Additionally, pySIPFENN can be set up for parallel computation and can be run on both personal machines and high-performance computers (HPC).

Young Calphadian Night

This is a traditional evening social event held during the annual CALPHAD conference. All attendees with a young mind are warmly invited to participate and have the opportunity to connect with fellow CALPHAD enthusiasts. A CALPHAD panel discussion will be organized, where attendees can gain insights into CALPHAD history, personal experiences, research anecdotes, and career development advice. Refreshments will be available, including drinks and snacks.

Time:

Wednesday, June 28th, Night event, 7:00-10:00 PM

Location:

Samberg Conference Center, 7th floor, Same room for the poster session.

Organizers:

- Wei Xiong, University of Pittsburgh, Associate Professor (CALPHAD Young Leader Awardee 2020)
- Richard Otis, NASA Jet Propulsion Laboratory, Technologist (CALPHAD Young Leader Awardee 2021)

Panelists:

- Charles Kuehmann, SpaceX / Tesla, Vice President Materials Engineering
- Greg Olson, MIT, Thermo-Calc Professor of the Practice
- Rainer Schmid-Fetzer, Clausthal University of Technology, Professor Emeritus
- Raymundo Arróyave, Texas A&M University, Professor

Information about CALPHAD Young Leader Award:

- <https://calphad.org/calphad-awards#CYLA>
- <https://calphad.org/Data/Sites/1/awards/bylaws-calphad-young-leader-award-2021.pdf>

Conference Agenda

Abstracts for each presentation can be found in the following section. To easily locate the abstract of each oral presentation, please refer to the presentation index number provided in the first column of the agenda table.

Important Notes:

*To ensure a smooth session, we kindly request that **all presentation files be saved on the conference laptop prior to the start of each session**. All files will be removed from the laptop after the conference. While we discourage using personal laptops due to time constraints, if necessary, please ensure that you test the projector connection well before the session start time.*

*There will be **two poster sessions** scheduled as follows:*

- *Poster Session 1: 7:00 - 10:00 PM, Monday, 6/26.
Please set up your poster by 2:00 PM on Monday and remove it by 12:00 PM noon on Tuesday.*
- *Poster Session 2: 7:00 - 10:00 PM, Tuesday, 6/27.
Please set up your poster by 2:00 PM on Tuesday and remove it by 12:00 PM noon on Wednesday.*

Should you have any inquiries or require assistance, please feel free to reach out to Yu Zhong, Wei Xiong, or any member of the organizing committee.

Session 1**June 26, 2023, Monday AM****Part I - CALPHAD: Past, Present, and Future***Chairs: Yu Zhong & Wei Xiong**Monday, Jun 26, 2023*

	08:00 – 08:10	Opening	Yu Zhong & Wei Xiong
O1	08:10 – 08:30	Materials Genomics: Honoring the Vision of Larry Kaufman	Greg Olson
O2	08:30 – 08:50	Mats Hillert and CALPHAD – a memorial tribute	John Ågren
O3	08:50 – 09:10	Towards the integration of quantum, statistical, and irreversible thermodynamics for accurate prediction of free energy landscape and kinetic properties	Zi-Kui Liu
O4	09:10 – 09:30	Developing Models and Software for 50 years	Bo Sundman
O5	09:30 – 09:50	3rd generation models – review and way forward	Malin Selleby
O6	09:50 – 10:15	CALPHAD for a Better Planet and an Interplanetary Future	Charles Kuehmann
	10:15 – 10:45	Coffee Break	

Part II - CALPHAD Modeling and Database Development (I)*Chairs: Rainer Schmid-Fetzer & Malin Selleby**Monday, Jun 26, 2023*

O7	10:45 – 11:05	Thermodynamic database for multi-principal element alloys within the system Al–Co–Cr–Fe–Mn–Ni–C(–V)	Bengt Hallstedt
O8	11:05 – 11:25	Thermodynamic assessment of ternary Al–M–O (M = Nb, Ta) systems	Julian Gebauer
O9	11:25 – 11:45	Thermodynamic prediction of the C-dependency for bainite formation: the importance of Fe–C	Aurélie Jacob

O10	11:45 – 12:05	Assessment on the Li-Ni-Mn-Co-O System and Applications on Lithium-Ion Batteries Layered Cathodes	Lucas Tosin Paese
O11	12:05 – 12:25	Development of QuesTek Databases for Integrated Computational Material Design	Zhi Liang

Lunch starts at 12:30 PM

Session 2 **June 26, 2023, Monday PM**

Part I - Atomistic Modeling and Prediction (I)

Chairs: André Costa e Silva & Jooho Lee

Monday, Jun 26, 2023

O12	14:00 – 14:20	Using ab-initio phase diagrams to tune experimental synthesis routes	Mira Todorova
O13	14:20 – 14:40	Construction of the Theoretical Phase Diagrams Based on the First-Principles Calculation	Hiroshi Ohtani
O14	14:40 – 15:00	Finite temperature boundary energy of Al	Shigeto Nishitani
O15	15:00 – 15:20	Ab Initio Modeling on The Thermodynamic and Temperature-Dependent Elastic Properties of Subsystems of The FCC FeNiCoCr Medium Entropy Alloys (MEAs)	Songge Yang
O16	15:20 – 15:40	High Temperature Al-Zn-Mg Alloys Design: High-throughput DFT Calculations and Machine Learning	Yu-ning Chiu
	15:40 – 16:10	Coffee Break	

Part II - CALPHAD Applications (I)

Chairs: Bengt Hallstedt & Dongwon Shin

Monday, Jun 26, 2023

O17	16:10 – 16:30	Lithium-ion Batteries Studied by Calorimetry and CALPHAD	Hans Jürgen Seifert
O18	16:30 – 16:50	Insights into improving steel secondary metallurgy using computational thermodynamics	André Costa e Silva

O19	16:50 – 17:10	Approaching Multiphysics Problems from Entropy	Ping Wu
O20	17:10 – 17:30	Validation and Application of the Genova High-Entropy Alloys (GHEA) Thermodynamic Database for Selected Multi-component Systems	Lorenzo Fenocchio
O21	17:30 – 17:50	Feasibility Map: A CALPHAD-Based Approach to Design Composition Pathway for Desired Dissimilar Materials Processed by Casting, Welding and Additive Manufacturing	Hui Sun

Dinner starts at 6:00 PM

Poster session (1) from 7:00 to 10:00 PM

Session 3 **June 27, 2023, Tuesday AM**

Part I - CHiMaD Sponsored session: Materials Genome and Materials Design (I)

Chairs: John Ågren & Sinn-wen Chen

Tuesday, Jun 27, 2023

O22	08:00 – 08:25	The Materials Genome Initiative: Reaching for Impact	James Warren
O23	08:25 – 08:45	CALPHAD models: quo vadis?	Ursula Kattner
O24	08:45 – 09:05	CALPHAD Uncertainty Quantification: Problems and Solutions	Noah Paulson
O25	09:05 – 09:25	CALPHAD Uncertainty Quantification and Design with Uncertainty	Changning Niu
O26	09:25 – 09:45	Shapes of Single-Phase Diagrams	Adetoye Adekoya
O27	09:45 – 10:05	A CALPHAD model of non-equilibrium plane-front and dendritic growth in concentrated multicomponent alloys	Christopher Hareland
	10:05 – 10:35	Coffee Break	

Part II - CHiMaD Sponsored session: Materials Genome and Materials Design (II)

Chairs: Qing Chen & Shih-kang Lin

Tuesday, Jun 27, 2023

O28	10:35 – 10:55	Development of a thermodynamic database for Co-based superalloys.	Pereira dos Santos Julio Cesar
O29	10:55 – 11:15	Printable Co Superalloys Exploiting Multiphase Precipitation Strengthening for Strain-Age Cracking Resistance	Krista Biggs
O30	11:15 – 11:35	Printable Die Steel for GigaCasting	Florian Hengsbach
O31	11:35 – 11:55	High-strength high-damping steels: A CALPHAD assisted alloy design study	Julian Rackwitz
O32	11:55 – 12:20	ICME applications in Pratt & Whitney	David Furrer

Lunch starts at 12:30 PM

Session 4

June 27, 2023, Tuesday PM

Part I - CALPHAD Applications (II)

Chairs: Soumya Sridar & Bi-Cheng Zhou

Tuesday, Jun 27, 2023

O33	14:00 – 14:25	Development of Grade 700 MPa High-Strength Seismic Rebars by Integrated Computational Materials Engineering and Machine Learning	Joonho Lee
O34	14:25 – 14:45	Physics-constrained, inverse design of high-temperature, high-strength, creep-resistant printable Al alloys using machine learning methods	S. Mohadeseh Taheri-Mousavi
O35	14:45 – 15:05	Modelling elemental surface sublimation of single crystal Ni-based superalloys at high temperatures	Dimitra Spathara
O36	15:05 – 15:25	CalPhaD-Assisted Alloy Design for Fe-based Shape Memory Alloys	Mario J. Kriegel
O37	15:25 – 15:45	Modelling reactions between ceramic oxides and Ti-Al melt	Joseph Moses
	15:45 – 16:15	Coffee Break	

Part II - CALPHAD Applications (III)

Chairs: Nils Warnken & Alexander Pisch

Tuesday, Jun 27, 2023

O38	16:15 – 16:35	High-throughput CALPHAD to Augment Scientific Features in Modern Data Analytics for Advanced Alloy Design	Dongwon Shin
O39	16:35 – 16:55	Alloy Data Quality Assurance Tools in ULtrahigh TEMperature Refractory Alloys (ULTERA) Database	Adam Krajewski
O40	16:55 – 17:15	Development of a thermodynamic database for future control of tramp elements in steelmaking processes	Michael Bernhard
O41	17:15 – 17:35	New feedstock design for additive manufacturing using a commercial alloy powder mixture	Daozheng Li
O42	17:35 – 17:55	High-Entropy Materials Design by Integrating the First-Principles Calculations and Machine Learning: A Case Study in the Al-Co-Cr-Fe-Ni System	Guangchen Liu

Dinner starts at 6:00 PM

Poster session (2) from 7:00 to 10:00 PM

Session 5

June 28, 2023, Wednesday AM

Part I - Experimental Equilibria and Phase Transformations

Chairs: Andre Schneider & Stephanie Lippmann

Wednesday, Jun 28, 2023

O43	08:00 – 08:20	How experimental thermochemistry can help actinide theory and phase equilibria.	Alexandra Navrotsky
O44	08:20 – 08:40	Enthalpy of mixing in entropy stabilised oxides	Scott McCormack
O45	08:40 – 09:00	Heat of dissolution & standard heat of formation of oxides using high temperature calorimetry	Alexander Pisch
O46	09:00 – 09:20	Eutectic and liquidus temperatures of Sn-based alloys	Sinn-wen Chen
O47	09:20 – 09:40	Structure and thermodynamics of ceramics above 2000°C	Sergey Ushakov

O48	09:40 – 10:00	Coupled Phase Diagram Experiment and Thermodynamic Modeling of the La_2O_3 -MgO-SiO ₂ System	Jeong-Min Cheon
	10:00 – 10:30	Coffee Break	

Part II - Atomistic Modeling and Prediction (II)

Chairs: Raymundo Arróyave & Theresa Davey

Wednesday, Jun 28, 2023

O49	10:30 – 10:50	Metastable defect phase diagrams as road map for defect design	Jörg Neugebauer
O50	10:50 – 11:10	Stability of FeNiCoCrMnAl _x and FeNiCoCrPdAl _x : fully disordering vs. partially disordering	Ying Chen
O51	11:10 – 11:30	Design metastability in high-entropy alloys by tailoring unstable fault energies	Wei Chen
O52	11:30 – 11:50	A Parameter-Free First-Principles-Based Debye Model to Predict Thermodynamic Properties of Complex Alloy Systems	Yi Wang
O53	11:50 – 12:10	Towards high throughput melting property calculations with ab initio accuracy aided by machine learning potential	Lifang Zhu

Lunch starts at 12:30 PM

Activities June 28, 2023, Wednesday PM

14:00	Excursion & social events: Duck Tour Boarding 2:00 PM.
17:15	Group photo in front of the MIT Great Dome (Check the map in the previous section for the standing point)
18:00	Dinner
19:00	Young Calphadian night

Session 6**June 29, 2023, Thursday AM****Part I - Diffusion and Phase Transformations***Chairs: Ping Wu & Karin Frisk**Thursday, Jun 29, 2023*

O54	08:00 – 08:20	From PE to OE: Cementite Precipitation Pathway in Steels	Qing Chen
O55	08:20 – 08:40	A Phase Field Model Based on Absolute Reaction Rate Theory	Nils Warnken
O56	08:40 – 09:00	Thermodynamic investigation on the formation of G.P. zone in the Al-Cu binary system	Takao Suzuki
O57	09:00 – 09:20	Beyond the parallel tangent method to predict composition of the first nucleating phase from oversaturated solutions	George Kaptay
O58	09:20 – 09:40	PLEIADES/ALCYONE simulations of irradiated fuel thermochemistry coupled with oxygen thermal diffusion	Clément Introïni
O59	09:40 – 10:00	Deep Learning for Large-Scale Prediction of Melting Temperature and Materials Properties	Qi-Jun Hong
	10:00 – 10:30	Coffee Break	

Part II - CALPHAD Modeling and Database Development (II)*Chairs: Scott McCormack & Dimitra Spathara**Thursday, Jun 29, 2023*

O60	10:30 – 10:50	3rd generation unary descriptions at high temperature	Rainer Schmid-Fetzer
O61	10:50 – 11:10	Uncertainty Quantification and Propagation in CALPHAD and CALPHAD-based Frameworks	Raymundo Arróyave
O62	11:10 – 11:30	Site occupancies in the quinary Co–Cr–Fe–Mn–Ni σ phase	Jean-Marc Joubert
O63	11:30 – 11:50	Calculation of Spinodal and Critical Point in Multicomponent Systems	Shuanglin Chen
O64	11:50 – 12:10	First-principles Thermodynamic Database for the Al-Ni-Ti	Arkapol Saengdeejing

Lunch starts at 12:30 PM

Session 7**June 29, 2023, Thursday PM****Part I - Thermodynamic Software and Model Development***Chairs: Shuanglin Chen & Ursula Kattner**Thursday, Jun 29, 2023*

O65	14:00 – 14:20	A virtual laboratory for the aluminum industry	Jean-Philippe Harvey
O66	14:20 – 14:40	The new Thermo-Calc Additive Manufacturing Module	Andre Schneider
O67	14:40 – 15:00	A Cluster-Based Computational Thermodynamics Framework with Intrinsic Chemical Short-Range Order	Bi-Cheng Zhou
O68	15:00 – 15:20	New strategies for thermodynamic equilibria in Calphad optimizations	Florian Tang
O69	15:20 – 15:40	Novel Model for Gibbs Free Energy and Conductivity in Space Charge Layers Utilizing the CALPHAD Method	Samuel Krimmel
	15:40 – 16:10	Coffee Break	

Part II - Thermodynamic Modeling, Database and Design Applications (I)*Chairs: Richard Otis & Zhi Liang**Thursday, Jun 29, 2023*

O70	16:10 – 16:30	Thermochemical Modeling of Nuclear Thermal Propulsion Fuel Materials	Gustavo Costa
O71	16:30 – 16:50	Thermodynamic modeling of LiCl-KCl-NaCl-UCl ₃ system facilitating molten salt electrolysis for reprocessing spent nuclear fuel	Soumya Sridar
O72	16:50 – 17:10	Thermodynamic database for zirconium alloys used in Pressurized Water Reactors	Tuan-Minh Vu
O73	17:10 – 17:30	Major revisions of the Si-Zr phase diagram	V. B. Rajkumar
	18:00	Depart from Hotel for Odyssey Dinner Cruise.	

Session 8**June 30, 2023, Friday AM****Part I - Thermodynamic Modeling, Database and Design Applications (II)***Chairs: Arkapol Saengdeejing & Aurélie Jacob**Friday, Jun 30, 2023*

O74	08:00 – 08:20	CALPHAD Design of New Alloys and the Importance of the Databases	Karin Frisk
O75	08:20 – 08:40	ICME-Accelerated Alloy Design and Property Prediction of Novel Austenitic Steel Strengthened by Nano-precipitates	Colin Stewart
O76	08:40 – 09:00	Iron tolerance in Mg-Ca-Zn-Mn Biomedical alloy with CALPHAD Driven Analysis	Thomas Avey
O77	09:00 – 09:20	Development of thermodynamic database for ZrO ₂ -Y ₂ O ₃ -HfO ₂ -Ta ₂ O ₅ -system	Manuel Löffler
O78	09:20 – 09:40	Machine Learning for Alloy Design and Optimization of Process Conditions	Jaemin Wang
O79	09:40 – 10:00	Construction of Phase and Defect Diagrams from a Spectral Regular Solution Model for Grain Boundary Segregation	Thomas Matson
	10:00 – 10:30	Coffee Break	

Part II - Thermodynamic Modeling, Database and Design Applications (III)*Chairs: Jean-Marc Joubert & Hans Jürgen Seifert**Friday, Jun 30, 2023*

O80	10:30 – 10:50	Applications of CALPHAD in modeling microstructure in casting and thermo-mechanical processing of steels	Chunhui Luo
O81	10:50 – 11:10	Temperature gradients for materials characterization	Stephanie Lippmann
O82	11:10 – 11:30	Experimental investigation and thermodynamic assessment of the Cr–Mo–Ti system	Agustin Flores
O83	11:30 – 11:50	Application of phase-field modeling to the recovery of Pt nanoparticles from spent automotive catalysts.	Hélène Verbeeck
O84	11:50 – 12:10	Materials Design in Additive Manufacturing Using ICME Modeling with High-Throughput Experimentation	Wei Xiong
	12:10 – 12:20	Closing remarks	Yu Zhong & Wei Xiong

A lunch box will be provided starting from 12:30 PM