CALPHAD 2026

53rd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry

June 7 – 12, 2026

Centre des congrès de Québec, Québec City, Canada

Preface

Dear colleagues and friends,

It is with great pleasure that we welcome you to Quebec City for the 53rd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry. We are honoured to host the CALPHAD community in this remarkable city, whose four centuries of history, French-rooted culture, and UNESCO-listed Vieux-Québec offer a fitting setting for a week of scientific exchange.

Since its first edition more than half a century ago, CALPHAD has brought together those who develop and apply thermodynamic and phase-diagram modelling to advance our understanding of materials. The 2026 edition continues this tradition with roughly 86 oral presentations and 53 posters, covering fundamental thermodynamic modelling, DFT-informed approaches, applications to metallic and oxide systems, machine-learning methods in CALPHAD, and the design of materials for energy and process industries. We are particularly pleased to see strong participation from junior researchers, whose work will shape the field in the years to come.

A conference of this scope is the product of many hands. We wish to thank the members of the Organizing and Scientific Committees for their dedication, our sponsors for their generous support, the staff of the Centre for Research in Computational Thermochemistry (CRCT) at Polytechnique Montréal, and the team at the Quebec Convention Centre. Above all, we thank each of you — speakers, poster presenters, and participants — for making the journey to Quebec City.

We invite you to make the most of the scientific programme, to renew old collaborations and to build new ones, and also to step outside and enjoy what the city has to offer: the cobblestone streets of the Petit-Champlain, the ramparts of the Citadelle, and the view of the St. Lawrence from Château Frontenac. *Bon congrès et bienvenue à Québec.*

Patrice Chartrand & Jean-Philippe Harvey
Conference Chairs, CALPHAD 2026

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Organizing Committee

Conference Chairs

Patrice Chartrand, Polytechnique Montréal
Jean-Philippe Harvey, Polytechnique Montréal

Organizing Committee Members

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Sponsors

CALPHAD 2026 gratefully acknowledges the support of our sponsors.

Program at a Glance

June 7 (Sun)	Registration from 13:00 | 18:30 (310 Hall)					13:00 | 17:00 **Workshop FactSage Laval University** ADJ-2320	13:00 | 17:00 **Workshop Pandat Laval University** ADJ-2300	13:00 | 17:00 **Workshop PyCalphad Laval University** ADJ-4512	18:30 | 20:00 **Welcome reception (pink coupon)** Espace Urbain		
June 8 (Mon)	7:15 **Breakfast** Espace Urbain	8:00 | 10:00 **Fundamental Thermo Modelling – 1** 306AB	10:00 | 10:20 **Break**	10:20 | 12:00 **CALPHAD Assisted Material Design of Metallic Systems – 1** 306AB	12:00 | 13:30 **Lunch** Espace Urbain	13:30 | 15:30 **Fundamental Thermo Modelling – 2** 306AB	15:30 | 15:50 **Break**	15:50 | 17:50 **DFT in CALPHAD** 306AB	17:50 | 19:20 **Dinner (blue coupon)** Espace Urbain	19:30 | 21:00 **Poster Session #1 (red coupon)** 308AB	21:00 | 22:30 **Young Calphadian Night** 306AB
June 9 (Tue)	7:15 **Breakfast** Espace Urbain	8:00 | 10:00 **Fundamental Thermo Modelling – 3** 306AB	10:00 | 10:20 **Break**	10:20 | 12:00 **CALPHAD Assisted Material Design of Metallic Systems – 2** 306AB	12:00 | 13:30 **Lunch** Espace Urbain	13:30 | 15:30 **Calphad Application - 1** 306AB	15:30 | 15:50 **Break**	15:50 | 17:50 **Calphad Application - 2** 306AB	17:50 | 19:30 **Dinner** Espace Urbain	19:30 | 21:00 **Poster Session #2 (orange coupon)** 309AB	20:30 | 22:30 **CALPHAD AGA (Board members only)** Room 311
June 10 (Wed)	7:15 **Breakfast** Espace Urbain	8:00 | 10:00 **Software and New Models** 306AB	10:00 | 10:20 **Break**	10:20 | 12:00 **CALPHAD for Aluminum Alloys** 306AB	12:00 | 13:30 **Lunch** Espace Urbain	13:30 | 14:00 **Group picture** Promenade Desjardins	15:30 | 17:30 Huron Traditional site	17:45 | 20:15 Cocktail and Meal at *La Sagamité*	18:15 Wendat Nation Conference & Wendat Song	20:30 | 21:00 Myths & Legends at Onhwa' Lumina	21:00 | 22:15 Onhwa' Lumina night walk
							Social excursion Wendake (Bus departure - **14:45** from the Delta Hotel)				
June 11 (Thu)	7:15 **Breakfast** Espace Urbain	8:20 | 10:20 **Diffusion, Microstructure, Properties** 306AB	10:20 | 10:40 **Break**	10:40 | 12:00 **CALPHAD for Oxides – 1** 306AB	12:00 | 13:30 **Lunch** Espace Urbain	13:30 | 14:50 **CALPHAD for Nuclear Applications** 306AB	14:50 | 15:10 **Break**	15:10 | 16:30 **CALPHAD for Salts** 306AB	18:00 | 22:30 Boarding 18:00 | Departure **19:00** Banquet Cruise (Awards announcement) Buses leave the Delta Hotel at 17:30 Chouinard Wharf, 10 Dalhousie Street, Québec, QC G1K 8L8		
June 12 (Fri)	7:15 **Breakfast** Espace Urbain	8:00 | 10:20 **CALPHAD Applications to Metallic Systems** 306AB	10:20 | 10:40 **Break**	10:40 | 12:00 **CALPHAD for Oxides – 2** 306AB	12:00 | 13:30 **Lunch boxes** 308-309 corridor						

Venue




Conference venue

Centre des congrès de Québec
1000 boulevard René-Lévesque Est
Québec, QC G1R 5T8, Canada

Conference hotel

Hôtel Delta Québec
690 boulevard René-Lévesque Est
Québec, QC G1R 5A8, Canada

Transportation

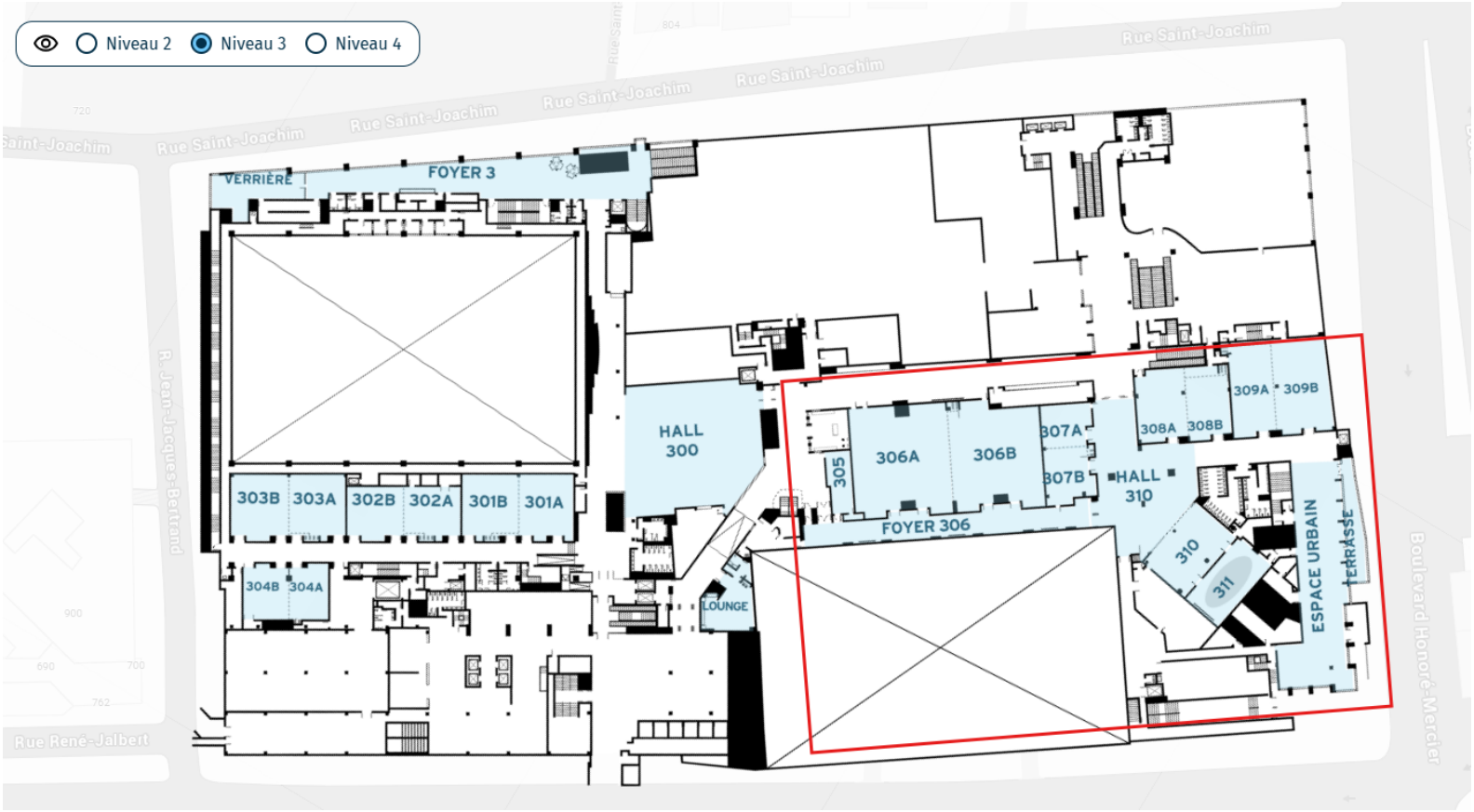
Taxis Coop 418-525-5191, Taxi Laurier 418-651-2727, Quebec City is also well deserved by Uber and Lyft.

Enjoy Your Badge Program

Throughout your stay, your CALPHAD 2026 badge unlocks exclusive offers at participating restaurants, museums, cultural attractions, boutiques and entertainment venues across Québec City. Simply present your badge at the point of purchase. A few establishments have specific conditions or codes – the full list of partners and offers is available at:

https://www.convention.qc.ca/en/plan-visit/enjoy-your-badge-program/

Floor map



Emergencies: each room has an emergency plan and a QR code that allows you to contact the Center's staff, who serve as first responders. The direct number is: **418-644-8796**.

City map

See the Official Calphad 2026 website for an interactive map with points of interest for the Calphad Conference.

Pre-conference Workshops

Three pre-conference workshops will be held on Sunday, June 7, 2026, at Université Laval (Pavillon Alphonse-Desjardins). All three sessions run from 13:00 to 17:00 and require separate registration.

Workshop | FactSage

FactSage is a fully integrated thermochemical database and software system widely used to calculate phase equilibria and thermodynamic properties of alloys, slags, salts, ceramics and aqueous solutions. This workshop presents practical and advanced uses of FactSage 8.4 together with ChemApp, the CALPHAD Optimizer, ThermML and database optimization examples, and closes with a FactFlow demonstration linking equilibrium calculations to process-level simulation. A short look at the new FactSage 9.0 installation approach is also included.

When: Sunday, June 7, 2026
Time: 13:00 – 17:00
Location: Université Laval, Pavillon Alphonse-Desjardins, Room ADJ-2320
Organizer: GTT-Technologies / CRCT
Instructors: Jean-Philippe Harvey, Christopher W. Bale, Kyota Poëti & Kentaro Oishi (CRCT, Polytechnique Montréal) — Moritz to Baben, Florian Tang & GTT team (GTT-Technologies)
Full program: FactSage_Workshop_Calphad_2026.pdf

A FactSage workshop version will be provided to registered participants before the workshop; installation instructions and any preparation steps will be sent in advance. Participants who wish to follow selected demonstrations on their own machines should bring a laptop; the session is also accessible to attendees who prefer not to run the software during the workshop.

Who should attend

- CALPHAD researchers, database developers, and materials scientists working with phase equilibria, high-temperature processes, alloy design, or process chemistry.
- Process-modelling researchers and industrial users connecting thermodynamic calculations with process-level analysis.
- Students, postdoctoral researchers, and new users seeking a structured introduction to FactSage, ChemApp, and FactFlow.
- Current FactSage users interested in the new FactSage 9.0 installation approach and recent additions to the suite.

Agenda

- Opening — FactSage, CRCT, and GTT-Technologies (13:00 – 13:15).
- FactSage 8.4 today — current capabilities and practical workflows (13:15 – 14:15).
- ChemApp, CALPHAD Optimizer, ThermML, and database optimization examples (14:15 – 15:05).
- Advanced equilibrium calculation example and FactFlow process-simulation demonstration (15:15 – 16:30).
- FactSage 9.0 installation approach, discussion and attendee feedback (16:30 – 17:00).

Workshop | Pandat

This workshop, organized by CompuTherm LLC, introduces Pandat as an integrated CALPHAD platform for materials design and process simulation. Participants will see how Pandat supports phase diagram calculations, thermodynamic analysis, precipitation and recrystallization modelling, diffusion simulation, and solidification analysis, with examples that emphasise practical workflows for research and accelerated materials development.

When: Sunday, June 7, 2026
Time: 13:00 – 17:00
Location: Université Laval, Pavillon Alphonse-Desjardins, Room ADJ-2300
Organizer: CompuTherm LLC
Instructors: Dr. Shuanglin Chen (CompuTherm LLC) — Prof. Rainer Schmid-Fetzer (TU Clausthal)
Full program: Pandat_Workshop_Calphad_2026.pdf

No advanced Pandat experience is required. Basic familiarity with materials thermodynamics, phase diagrams and heat-treatment or solidification concepts is helpful. Participants are encouraged to install the Pandat education version (Pandat_2026_Education_Setup.exe) before the workshop.

Who should attend

- Researchers, engineers, and industry practitioners using computational thermodynamics, alloy design, phase transformation, or process modelling.
- Graduate students, postdoctoral researchers, and new users seeking a practical introduction to Pandat.
- Current Pandat users interested in recent features and broader applications.

Agenda

- Introduction — development of Pandat software.
- Pandat overview — interface, workflow, modules, and databases.
- Live demonstration — Pandat simulation and result interpretation.
- Discussion — questions, applications, and more.

Workshop | Open-source CALPHAD tools (PyCalphad, ESPEI, Kawin)

This workshop gives a detailed introduction to CALPHAD-type computational thermodynamics and kinetics software within the PyCalphad ecosystem. It features hands-on exercises in an interactive cloud environment that enables attendees to calculate phase diagrams, simulate solid-state precipitation in alloys, and propagate uncertainty in thermodynamic calculations. Attendees are encouraged to bring a laptop or computing device to follow along interactively. Tables, power outlets, and Wi-Fi will be provided.

When: Sunday, June 7, 2026
Time: 13:00 – 17:00
Location: Université Laval, Pavillon Alphonse-Desjardins, Room ADJ-4512
Components: PyCalphad — ESPEI — Kawin
Audience: Engineers and practitioners interested in open-source materials-design tools.
Full program: PyCalphad_Workshop_Calphad_2026.pdf

Agenda

13:00 | Opening and introductions
13:15 | PyCalphad
14:15 | ESPEI
15:15 | Break
15:30 | Kawin
16:30 | Discussion and Q&A
17:00 | Closing

Social activities

Excursion | Wendake, La Sagamité & Onhwa' Lumina night walk

The Wendat — historically called Huron in French colonial records — are a First Nation whose ancestral homeland includes Wendake, a community located just minutes north of Quebec City. This excursion immerses participants in their culture: the Huron-Wendat Traditional Site introduces ancestral knowledge and daily life; dinner is served at *La Sagamité*, a restaurant named after a traditional Wendat corn-and-bean stew; and the evening concludes with *Onhwa' Lumina*, an outdoor night walk through the forest celebrating Wendat stories, song, and connection to the land.

When: Wednesday, June 10, 2026
Cost: Included
Starting point: Delta Hotel
Destination: Wendake

14:45 | Departure

Private bus transfer to the Huron Traditional Site.

15:30 – 17:30 | Huron Traditional Site

Activities: walk through a reconstructed 17th-century Wendat village including a traditional longhouse, smokehouse, and sweat lodge; observe demonstrations of ancestral knowledge such as traditional transportation (canoes, snowshoes), hunting techniques, and traditional medicine; enjoy a hands-on experience of Wendat daily life, taking in the wood smoke, traditional furs, and village architecture.

17:30 | Private bus transfer to La Sagamité restaurant

17:45 – 20:15 | Dinner at La Sagamité

A refined three-course dinner inspired by traditional Wendat cuisine, served in a warm and welcoming atmosphere. The evening includes a presentation by the Wendat Nation and a traditional song.

18:15 | Wendat Nation Conference & Wendat Song

20:15 | Private bus transfer to Onhwa' Lumina

20:30 – 21:00 | Myths & Legends at Onhwa' Lumina

An intimate storytelling experience by the fire in the Ekionkiestha' Longhouse, where traditional stories about the creation of Mother Earth, the Pleiades, and other ancestral myths offer a unique insight into Huron-Wendat culture.

21:00 – 22:15 | Onhwa' Lumina Night Walk

An enchanting night walk celebrating the Huron-Wendat Nation. Under the stars, experience ancestral rhythm and song within the Great Circle, fostering a sense of connection with all living things.

22:15 | Private bus transfer to the Delta Hotel

Accompanying Persons | Monday June 8: Culture & Green Space

When: Monday, June 8, 2026
Cost: Free
Starting point: Québec Convention Centre
Destination: Grande Allée, Plains of Abraham, Old Québec, Château Frontenac
Theme: History, scenery, and iconic Québec landmarks. Timing may vary based on the group's pace and energy levels.

08:30 | Departure from Québec Convention Centre

Begin on foot toward Grande Allée.

08:35 – 09:00 | Grande Allée (25 min)

Highlights: Historic façades, cafés, and lively atmosphere.
Experience: Quick coffee or light breakfast stop.

09:05 – 10:15 | Plains of Abraham (1 h 10)

Must-visit: Joan of Arc Garden, Martello Towers, river viewpoints.
Highlights: Historic 1759 battlefield, scenic walking paths, panoramic views.
Experience: Relaxing walk combining history and nature.

10:15 – 10:30 | Walk to Old Québec

Scenic downhill route with views of the fortifications.

10:30 – 11:15 | Old Québec (45 min)

Must-visit: Place d'Armes, city walls, Terrasse Dufferin.
Highlights: UNESCO World Heritage Site with European charm.
Experience: Explore cobblestone streets and the historic ambiance.

11:15 – 11:45 | Château Frontenac & Dufferin Terrace (30 min)

Must-visit: Château exterior / lobby, terrace boardwalk.
Highlights: Iconic landmark, river views, photography spots.
Experience: Enjoy views, take photos, optional short break.

12:00 | Return to Québec Convention Centre

Accompanying Persons | Tuesday June 9: Nature & Excursion

When: Tuesday, June 9, 2026
Cost: Free
Starting point: Québec Convention Centre
Destination: Montmorency Falls Park, Île d'Orléans
Theme: Nature, countryside scenery, and local flavours. Timing may vary depending on pace and traffic.

Morning program — Montmorency Falls Park (08:30 – 11:30)

08:30 | Departure from Québec Convention Centre

08:50 – 10:50 | Montmorency Falls Park

Address: 5300 Boulevard Sainte-Anne, Québec, QC
Highlights: 83 m waterfall (higher than Niagara Falls), suspension bridge, cable car, scenic trails.
Must-visit: Main lookout, suspension bridge, cable car station.

11:30 | Return to Québec Convention Centre

Afternoon program — Île d'Orléans scenic tour (13:30 – 17:30)

Reference: https://www.quebec-cite.com/en/what-to-do-quebec-city/tour-ile-orleans

13:30 | Departure from Québec Convention Centre

14:00 – 14:50 | Vignoble Ste-Pétronille

Address: 8705 Chemin Royal, Sainte-Pétronille, QC
Highlights: Panoramic Québec City views, wine / cider tasting, group photos.

15:00 – 15:45 | Chocolaterie de l'Île d'Orléans

Address: 1505 Chemin Royal, Saint-Pierre, QC
Highlights: Handmade chocolates, relaxing indoor stop.

15:45 – 16:15 | Church of Saint-Jean de l'Île d'Orléans

Address: 4623 Chemin Royal, Saint-Jean-de-l'Île-d'Orléans, QC G0A 3W0
Highlights: Historic village church.

16:15 – 16:50 | Mauvide-Genest Manor, lighthouse and Saint-Jean-de-l'Île-d'Orléans

Address: 2 Chemin du Quai, Saint-Jean-de-l'Île-d'Orléans, QC
Highlights: Traditional houses, authentic Québec charm.

17:30 | Return to Québec Convention Centre

Accompanying Persons | Thursday June 11: Family Activity and Parliament of Quebec

When: Thursday, June 11, 2026
Cost: Free
Starting point: Québec Convention Centre
Destination: National Museum of Fine Arts of Quebec (MNBAQ), Parliament of Quebec

Morning program — National Museum of Fine Arts of Quebec (MNBAQ)

09:00: Departure from Québec Convention Centre.

09:30 – 11:30 | National Museum of Fine Arts of Quebec (MNBAQ)

Quebec and Canadian art collections.
Contemporary exhibitions.

Afternoon program — Parliament of Quebec

14:00 – 15:30 | Parliament of Quebec

Historic government building.
13:30: Departure from Québec Convention Centre.
14:00: Arrival at the Parliament (security, registration, coat check, etc.).
14:30: Guided visit.
15:30: End of the visit.

Oral Presentations

Monday

Fundamental Thermo Modelling – 1

Chairs: J.-M. Joubert & A. Jacob

8:00-8:20 O1.1

A Unified Thermodynamic Framework: From Equilibrium and Nonequilibrium to Zentropy, Cross Phenomena, and Artificial Intelligence

Z.-K. Liu
Pennsylvania State University, United States of America

8:20-8:40 O1.2

Recursive entropy in thermodynamics: establishing the statistical-physics basis of the zentropy approach

L. Myers, N. Hew, S. Shang, Z. Liu
Pennsylvania State University, United States of America

8:40-9:00 O1.3

Thermodynamic Entropy as Information - A compression-based demonstration of the Shannon—Boltzmann equivalence in condensed matter

D. Fisher, Q.-J. Hong
Arizona State University, United States of America

9:00-9:20 O1.4

CALPHAD Coupled Integrated Computational Materials Engineering (ICME) Framework for Microstructure Evolution and Property Optimization

K. L. M. Elder, S. M. Peters, J. Kaipainen, G. E. Isitman, S. A. Khairallah, M. R. Tupek, B. Bocklund, D. A. Tortorelli, J. D. Roehling, S. Watts, J. L. Fattebert, J. T. McKeown, T. Andersson, A. Laukkanen, T. Pinomaa, A. Perron, H. Villanueva
Lawrence Livermore National Laboratory, United States of America

9:20-9:40 O1.5

High-throughput calculation of eutectic compositions

K. E. Borowski, K. Firdova, G. Deffrennes, J.-M. Joubert
Université Paris-Est Créteil, France

9:40-10:00 O1.6

The Calfateria

N. Dupin, S. G. Fries
Calcul Thermodynamique, France

CALPHAD Assisted Material Design of Metallic Systems – 1

Chairs: W. Xiong & R. Schmid-Fetzer

10:20-10:40 O1.7

Development of Thermodynamic Databases Coupled to Alloy Design of Metallic Materials

K. Frisk
Innomat AB, Sweden

10:40-11:00 O1.8

Model Development and Design of High Strength, High Toughness Naval Steels: 10Ni-150

Y. N. Lee, C. C. Tasan, G. B. Olson
Massachusetts Institute of Technology, United States of America

11:00-11:20 O1.9

CALPHAD-assisted design of high-performance titanium alloys and refractory materials for melting

H. Zhu, Q. Feng, P. Gao, G. Chen, C. Li
Shanghai University, China

11:20-11:40 O1.10

Constrained Target Function for Alloy Design

S. Chen, C. Zhang, W. Cao, F. Zhang
CompuTherm, LLC, United States of America

11:40-12:00 O1.11

Revisiting the Fe-Mo System: Structural Investigation and Thermodynamic Modeling of Frank-Kasper Phases

A. Flores, S. Chatain, P. Fossati, J.-M. Joubert
CEA Paris-Saclay, France

Fundamental Thermo Modelling – 2

Chairs: N. Dupin & B. Bocklund

13:30-13:50 O1.12

Optimization and Uncertainty Quantification of CALPHAD Model Parameters via the No-U-Turn Sampler

C. Kunselman, B. Bocklund, R. Otis, R. Arroyave
Texas A&M University, United States of America

13:50-14:10 O1.13

Efficient CALPHAD coupling of quasi-equilibrium thermodynamics using a hash-table-based extrapolation scheme

H. H. Y. Craven, N. Warnken
University of Birmingham, United Kingdom

14:10-14:30 O1.14

Calphad assessment strategy and unexpected liquid miscibility gaps

R. Schmid-Fetzer, C.-H. Ho, H.-C. Huang, S.-W. Chen
Clausthal University of Technology, Germany

14:30-14:50 O1.15

Comparison of different model equations for size- and shape-dependent integral and partial molar Gibbs energies of nano-phases to screen out the incorrect ones

G. Kaptay
University of Miskolc, Hungary

14:50-15:10 O1.16

A modified Scheil approach for nucleation-dependent solidification pathways

S. Y. Kwon, Y. Yang, A. Plotkowski, M. Rolchigo, A. Shyam, S. Bahl, N. A. Richter, J. A. Haynes
Oak Ridge National Laboratory, United States of America

15:10-15:30 O1.17

Developing reliable Calphad descriptions: lessons from the Fe-Ni system

Z. He, Q. Chen, M. Selleby
Swerim, Sweden

DFT in CALPHAD

Chairs: B. Hallstedt & Y. Zhong

15:50-16:10 O1.18

Using Universal Machine Learning Potential to Accelerate the Thermodynamic Database Development

A. Saengdeejing, R. Sahara, H. Kino, T. Chkyow
National Institute for Materials Science, Japan

16:10-16:30 O1.19

A hybrid methodology based on first-principles calculations and Calphad to predict the Ni-Co phase diagram incorporating configurational, vibrational and magnetic contributions

C. Shi, W. Shao, J. LLorca
Fundación IMDEA Materiales, Spain

16:30-16:50 O1.20

Overestimation of Silica Melting at Ambient Pressure in DFT and High-Accuracy MLIPs: Tackling Unreachable Relaxation Timescales

L.-F. Zhu, F. Körmann, A. Forslund, J. Neugebauer, B. Grabowski
University of Stuttgart, Germany

16:50-17:10 O1.21

Application of an uncertainty quantification method based on a heterogeneous ensemble of pretrained Universal machine learning interatomic potentials applied to steels with tramp elements

N. K. Mohandas, K. Liu, M. H. F. Sluiter
University of Technology Delft, Netherlands

17:10-17:30 O1.22

Ab Initio Prediction of the Magnetic Thermodynamics of LaCoO3 Perovskite Based on the Zentropy Theory

S. Yang, Y. Zhong
Worcester Polytechnic Institute, United States of America

17:30-17:50 O1.23

Automated computation of ab initio bulk and defect phase diagrams

A. Tehranchi, P. Mathews, J. Janßen, T. Hickel, J. Neugebauer
Max Planck Institute for Sustainable Materials, Germany

Tuesday

Fundamental Thermo Modelling – 3

Chairs: B.J. Lee & A. Saengdeejing

8:00-8:20 O2.1

Bayesian Design of Experiments for Calphad Modeling

B. Bocklund, I. R. Crystal, E. Sobalvarro Converse
Lawrence Livermore National Laboratory, United States of America

8:20-8:40 O2.2

Utilizing CALPHAD databases for alloy microstructure prediction via phase-field modeling

T. Morino, M. Ode, S. Hirosawa
Yokohama National University, Japan

8:40-9:00 O2.3

Toward Defect Phase Diagrams by Integrating Constraints into CALPHAD

M. to Baben, P. Matthews, K. Rejiba, T. Hickel, U. Kerzel, A. Walnsch
GTT Technologies, Germany

9:00-9:20 O2.4

Thermodynamic Modeling of Pure Elements with Quantitative Model Selection and Uncertainty Quantification using PyCalphad and ESPEI

A. Richter, I. Roslyakova, A. M. Beese, Z-K. Liu
The Pennsylvania State University, United States of America

9:20-9:40 O2.5

A Cluster-Based Computational Thermodynamics Framework with Intrinsic Chemical Short-Range Order: New Developments and Implications for Precipitate Nucleation Kinetics

H. Chen, B.-C. Zhou
University of Virginia, United States of America

9:40-10:00 O2.6

Calphad models for the liquid phase

B. Sundman, A. Flores, L. Kjellqvist, C. Guéneau
OpenCalphad, Sweden

CALPHAD Assisted Material Design of Metallic Systems – 2

Chairs: K. Frisk & M. Sluiter

10:20-10:40 O2.7

Combinatorial Additive Manufacturing–Enabled Materials Discovery and Modeling of W–Re–Os Alloys

W. Chen
University at Buffalo, United States of America

10:40-11:00 O2.8

Development of a high-throughput approach to assess oxidation resistance using chemically graded Ni-based superalloys

S. Ghanes, M. Degeiter, E. Epifano, T. Vaubois, F. Fossard, J. S. Mérot, N. Horezan, M. Perrut, D. Monceau
ONERA, France

11:00-11:20 O2.9

Evaluation of the Cu-Ti phase diagram and thermodynamic prediction of continuous and discontinuous precipitation

I. Ohnuma, T. Suzuki, H. Ohtani
National Institute for Materials Science, Japan

11:20-11:40 O2.10

Phase diagrams of Bi-Cu-Sn-Te quaternary system

C.-H. Ho, H.-C. Huang, C. Y. Chuang, Y.-C. Tsai, C.-Y. Hsieh, S.-W. Chen
National Tsing Hua University, Taiwan

11:40-12:00 O2.11

Materials design of high-strength, ultra-pure copper alloys for the next-generation detectors to unravel the nature of dark matter

D. Spathara, P. Knights, K. Nikolopoulos
University of Birmingham, United Kingdom

CALPHAD Applications – 1

Chairs: M. to Baben & B. Davis

13:30-13:50 O2.12

Thermodynamic and Kinetic Modelling of Oxide-Metal Reactions During Casting of Reactive Alloys

J. Moses, N. Warnken
University of Birmingham, United Kingdom

13:50-14:10 O2.13

Schaeffler diagram – a CALPHAD-view on an established application tool

A. Schneider
Thermo-Calc Software AB, Sweden

14:10-14:30 O2.14

Deoxidation Equilibria in Liquid Alloys

M.-K. Paek, G. Hils, Y.-B. Kang, I.-H. Jung
Clausthal University of Technology, Germany

14:30-14:50 O2.15

Integration of thermodynamics with process development in ferroalloy production

B. Davis, J.-P. Harvey
Kingston Process Metallurgy Inc., Canada

14:50-15:10 O2.16

An assessment of hydrogen-induced NiTi martensite transition

G. Pollini, E. Alvares, B. Bocklund, M. Palumbo, P. Jarebek, C. Pistidda
University of Turin, Italy

15:10-15:30 O2.17

Investigation of the effects of tramp elements on the pearlitic transformation for a sustainable steelmaking industry

A. Maille, J. Bouquerel, P. Antoine, M. Bonvalet Rolland
Centrale lille institut, France

CALPHAD Applications – 2

Chairs: I.H. Jung & T. Morino

15:50-16:10 O2.18

Thermodynamic Modelling of Protective Coating for Solid Oxide Electrolysis Cells

M. Saab, C. Guéneau, S. Chatain, P. V. B. Pinho
Commissariat énergie atomique et alternatives, France

16:10-16:30 O2.19

Modelling and probing solid solution-aqueous solution equilibria of aqueous nickel iron sulfate at 6 °C

J. Self, E. D. D. Da Silva, K. Oishi, J.-P. Harvey
Polytechnique Montréal, Canada

16:30-16:50 O2.20

Unexpected Cracking in WAAM Cu-Ni Deposited on Steel Base Plates: Understanding the Role of Fe

T. Avey, E. Holcombe, J. Norkett, J. Semple, C. Fisher
NSWC Carderock, United States of America

16:50-17:10 O2.21

Blast Furnace Simulation Using a CASCADE Framework and ChemApp for Python

A. Mansy, K. H. Spitzer, M. K. Paek
Technical University of Clausthal, Germany

17:10-17:30 O2.22

Modelling of inorganic solid phases formed during pyrogasification of biomass

D. A. Pinto Huanaco, J. H. Ferrasse, O. Boutin, L. M. Romero Millan, M. Hervy, Y. Kara
Aix Marseille University, France

17:30-17:50 O2.23

Machine learning-assisted crystal plasticity modeling of microcrack behavior in gradient-structured steels

X. X. Luo, C. K. Liu, S. Y. Wen, H. Mao, L. Y. Liu, X. Y. Zheng, Y. Du
Central South University, China

Wednesday

Software and New Models

Chairs: B. Sundman & C. Bale

8:00-8:20 O3.1

Thermodynamic Modeling of Metal Hydrides: Workflows, Software, and Applications to Multicomponent Databases

P. Hannappel, G. H. Gu, M. T. Curnan, Ł. Gondek, J. Czub, F. Heubner, M. Balcerzak, T. Weißgärber
TUD Dresden University of Technology, Germany

8:20-8:40 O3.2

PhaseForge: Automated CALPHAD-Compatible Phase Diagram Generation Using Universal Machine Learning Potentials

D. Sarıtürk, S. Zhu, R. Arróyave
Texas A&M University, United States of America

8:40-9:00 O3.3

Web-Based APIs for Automated Thermodynamic Property Generation: MAPP and SLUSCHI

Q.-J. Hong
Arizona State University, United States of America

9:00-9:20 O3.4

Building Interoperable CALPHAD Workflows: ThermML and Calphad Optimizer 3.0

F. Tang, B. Reis, M. to Baben
GTT Technologies, Germany

9:20-9:40 O3.5

FactFlow-Assisted Optimization of Aluminum Recycling Processing Balancing Economic Performance, Product Quality, and Environmental Impact

K. Poëti, D. Wei, K. Oishi, J-P. Harvey
Polytechnique Montréal, Canada

9:40-10:00 O3.6

Development of a Modified Polyhedron Model for Improved Estimation of Thermodynamic Properties of Mixed Oxides

E. Moosavi-Khoonsari, J. Arias Hernandez, S.-Y. Kwon
École de technologie supérieure, Canada

CALPHAD for Aluminum Alloys

Chairs: A. Kroupa & E. Povoden

Special Focus on Canadian Aluminum Research and Innovation

This session highlights CALPHAD applications for aluminum alloy development and acknowledges the valued support of **CQRDA** and **Hatch** in promoting aluminum research, innovation, and industrial collaboration in Canada.

10:20-10:40 O3.7

CALPHAD-driven discovery and rapid experimental validation of low-cost, high-strength, Al-alloys for additive manufacturing

B. Glaser, A. J. Hart, S. M. Taheri-Mousavi
Carnegie Mellon University, United States of America

10:40-11:00 O3.8

Thermodynamic modeling of the Al-rich Al-B system with LIBS/DSC Liquidus measurements

J.-R. Castillo-Sánchez, A. Vázquez Prudencio, P. Lafaye, J.-P. Harvey, K. Leosson, G. Salloum-Abou-Jaoude
Polytechnique Montréal, Canada

11:00-11:20 O3.9

Comparative Assessment of Crack Susceptibility Criteria Using Calphad Solidification Modeling and Graded Thermal Experiments

L. F. L. Pizano, W. Xiong
University of Pittsburgh, United States of America

11:20-11:40 O3.10

Molecular dynamics (MD) simulations of the nucleation of aluminum on TiB_2 interfaces with equivariant machine learning interatomic potentials (MLIAP)

D. Defrance, J-P. Harvey
Polytechnique Montréal, Canada

11:40-12:00 O3.11

CALPHAD assisted microstructural design to control precipitate and dispersoid evolution for improved strengthening in Al-Mg-Si-based alloys

S. K. Deb, A. Arora
Indian Institute of Technology Gandhinagar, India

Thursday

Diffusion, Microstructure, Properties

Chairs: Z.K. Liu & D. Larouche

8:20-8:40 O4.1

Thermodynamics and Diffusion Kinetics in Mn2Ti-type Hydrogen Storage Alloys

B.-J. Lee, J.-S. Lee, S.-H. Oh
Pohang University of Science and Technology, Korea (Republic of)

8:40-9:00 O4.2

Incorporation of molar volumes of diffusing elements in Onsager-type formulations of diffusion in alloys

A. R. khorasgani, S. Divinski, J. Kundin
Ruhr University Bochum, Germany

9:00-9:20 O4.3

The Thermodynamics of Planar Defects in Magnesium Alloys

P. Mathews, J. Janßen, A. Tehranchi, J. Neugebauer, T. Hickel
Federal Institute for Materials Research and Testing, Germany

9:20-9:40 O4.4

A predictive surface tension for liquid metallic solutions

Y. Kang, I.-H. Jung
Seoul National University, Korea (Republic of)

9:40-10:00 O4.5

Physics-based Thermal Conductivity Model Compatible with Multi-component CALPHAD Descriptions

Z. Liang, U. R. Kattner, M. J. Luebbe, F. Zhang, J. Martin, D. Kirsch, S. Chen
National Institute of Standards and Technology, United States of America

10:00-10:20 O4.6

Modelling Na–Mn–O cathodes and predicting cathode–electrolyte interface reactions for sodium-ion batteries

E. Povoden-Karadeniz, A. Khan, M. C. Poletti
Institute of Materials Science and Technology, Austria

CALPHAD for Oxides – 1

Chairs: E. Moosavi-Khoonsari & M. Perrut

10:40-11:00 O4.7

Systematics and thermodynamic modeling of the AEO-B2O3 (AE = Mg, Ca, Sr, Ba) binary systems

A. Pisch, N. Bouzid
Université Grenoble Alpes, France

11:00-11:20 O4.8

Revisiting RE-Ba-Cu-O Thermodynamics: From YBCO to Modern Gd- and Eu-Based Bulk Superconductors

D. Sedmidubský
University of Chemistry and Technology Prague, Czechia

11:20-11:40 O4.9

Thermodynamic Database Development for the Al2O3–CaO–MgO–SiO2–Fe2O3–FeO System and Its Application to Industrial Solid-Waste Utilization

F. Gao, Y. Liu, Hans J. Seifert, Y. Du
Central South University, China

11:40-12:00 O4.10

Thermodynamic Modelling of the CaO-MgO-SiO2 ternary system and its use in Ordinary Portland Cement Clinker Production

R. Bandak, W. R. Leal da Silva, A. Pisch
Université Grenoble Alpes, France

CALPHAD for nuclear applications

Chairs: S. Chen & P. Lafaye

13:30-13:50 O4.11

Software and Database Development for Design of Radiation-Resistant Alloys

N. Ury, B. Bocklund, N. Bertin, A. Perron
Lawrence Livermore National Laboratory, United States of America

13:50-14:10 O4.12

Enhancing Nuclear Reactor Safety: Thermodynamic Modelling of the Ag-Zr System in PWR Absorber Rods

C. Antion, M. Barrachin, P. Benigni, I. Crassous, A. Decreton, E. Fischer, S. Gyasi, A. Janghorban, M. Lomello, G. Mikaelian, I. Nuta, J. Rogez
University Grenoble Alpes, France

14:10-14:30 O4.13

Molten Salts Thermophysical Properties modelling: new insights into the effect of fission products accumulation in molten fuel salt systems

J. J. Soppo, O. T. Noordhuis, D. C. Alders, S. Couweleers, J. Vlieland, G. Pireddu, A. Salcedo, L. Ruszczynski, R. J. M. Konings, A. L. Smith
Delft University of Technology, Netherlands

14:30-14:50 O4.14

Thermodynamic Modeling of Phase Stability in Alloys under Irradiation

Y. Lu, C. Wang, X. Liu
Xiamen University, China

CALPHAD for Salts

Chairs: D. Lindberg & M. Saab

15:10-15:30 O4.15

Thermodynamic modeling and phase characterization in the Li2SO4-CoSO4-MnSO4-NiSO4 system for metal recovery from secondary resources

D. Lindberg, D. Sibarani, J. Biswas, G. Tewari, L. Klemettinen
Åbo Akademi University, Finland

15:30-15:50 O4.16

New thermodynamic model for salt-metal liquid solutions introducing charge defects within the CALPHAD approach

O. Kidari, P. Chartrand
Polytechnique Montréal, Canada

15:50-16:10 O4.17

Crystal Growth and Thermodynamic Assessment of the Thallium Alkaline-Earth Halides

E. van Loef, M. Inniss, M. Gillespie, K. Pestovich, L. Stand, L. S. Pandian, M. Zhuravleva
Radiation Monitoring Devices, Inc., United States of America

16:10-16:30 O4.18

Thermodynamic models for ternary deep eutectic systems

L. P. Zini, G. Teixeira, J.-P. Harvey, J. A. P. Coutinho, C. Robelin
Polytechnique Montréal, Canada

Friday

CALPHAD Applications to Metallic Systems

Chairs: U. Kattner & M. Selleby

8:00-8:20 O5.1
Understanding deformation-induced nanocrystallization in amorphous alloys: a multi-scale modeling study
S.-H. Oh, M. Wakeda
National Institute for Materials Science, Japan

8:20-8:40 O5.2
Liquidus projection of Cu-Se-Te ternary system
S.-W. Chen, C.-Y. Chung, Y.-C. Tsai, Y.-J. Chuang
National Tsing Hua University, Taiwan

8:40-9:00 O5.3
Phase-field modeling of austenitic fraction formation during tempering of 13Cr-4Ni martensitic stainless steels.
S. Valtierra, D. Paquet, V. Timoshevskii, D. Thibault, J-P. Harvey
Polytechnique Montréal, Canada

9:00-9:20 O5.4
Thermodynamic modelling of the Al–Ni–V system
B. Hallstedt, M. Noori
RWTH Aachen University, Germany

9:20-9:40 O5.5
Predictive thermodynamic modeling of the Suzuki effect in Co-Ni based alloys
A. Jacob, V. Razumovskiy, F. Moitzi, A. Robisson, E. Kozeschnik
TU Wien, Austria

9:40-10:00 O5.6
Optimizing Hardmetal Alloy Design Through CALPHAD and Experimental Investigation
T. Soria-Biurrun, S. Sridar, K. Frisk, L. Muñoz-Ortuño, F. Ibarreta-López, R. Martínez-Pampliega, J. M. Sánchez-Moreno
CEIT-BRTA, Spain

10:00-10:20 O5.7
Phase diagrams of Cu-Co-Sb ternary system
Yung-Chun Tsai, Ching-Yu Chuang, Cheng-Hsi Ho, Sinn-wen Chen
National Tsing Hua University, Taiwan

CALPHAD for Oxides – 2

Chairs: A. Pisch & D. Sedmidubský

10:40-11:00 O5.8
Gd3Sc2Al3O12 garnet scintillator: defect engineering
J. Ježek, J. Pejchal, D. Sedmidubský, P. Zemenová, V. Laguta, V. Babin, V. Jarý, A. Beitlerová, R. Kučerková, M. Nikl
Institute of Physics of the Czech Academy of Sciences, Czechia

11:00-11:20 O5.9
Thermodynamic Assessment of the Ba—Ti—O Ternary System
A. Albaalbaky, C. Gueneau, P. V. Borges Pinho
French Alternative Energies and Atomic Energy Comm., France

11:20-11:40 O5.10

Thermodynamic modeling of the CaO-Al2O3-P2O5-H2O system and applications to refractory materials design under H2-H2O conditions

G. Pei, I.-H. Jung
The University of Warwick, United Kingdom

11:40-12:00 O5.11

Development of a thermodynamic database for antimony oxide-containing metallurgical systems

A. Ahmadi Siahboumi, E. Moosavi-Khoonsari
École de technologie supérieure, Canada

Poster Presentations

Monday

Poster Session #1 - June 8, 19:30-21:00, Room 308/309AB

P1.1
Deep Alloy®: A New Frontier in Material Discovery
N. Adrián, Y. Fan, Y. Zhong
Worcester Polytechnic Institute, United States of America

P1.2
Thermodynamic model for sodium and potassium chromates, molybdates, and tungstates involved in high-temperature steel corrosion
S. Benalia, F. Tesfaye, D. Lindberg, L. Hupa, P. Chartrand, C. Robelin
Polytechnique Montréal, Canada

P1.3
Predicting thermal conductivity of graphite cathode blocks for aluminum electrolysis cells: A modeling approach
I. D. Bouzaine, P. Chartrand
Polytechnique Montréal, Canada

P1.4
Thermodynamic properties measurement of CaNdAl3O7 and CaNdAlO4
Y. Ma, S. Li, W. Wei, B. Yan, Z. Cao
University of Science and Technology Beijing, China

P1.5
Liquidus projection of the Cr-Nb-Ta system
V. M. Silveira, J. V. Luiz, K. E. Borowski, C. S. Barros, V. M. Chad, J. C. J. Gigolotti, C. A. Nunes, G. C. Coelho
University of São Paulo, Brazil

P1.6
Thermodynamic Modeling of the NaF-AlF_3-CaF_2-Al_2O_3-FeF_2-FeO-FeF_3-Fe_2O_3 System for Aluminum Production Using Inert Anodes : Experimental Study of the Fe-O-F Sub-System
C. V. d. S. Lima, P. Chartrand, C. Robelin
Polytechnique Montréal, Canada

P1.7
Thermodynamic and Microstructural Analysis of Lead-free Sn–Ag–Cu–Ga–Ni Solders
P. Danišovičová, I. Černičková, L. Ďuriška, R. Čička, T. Peričková
Slovak University Of Technology In Bratislava, Slovakia

P1.8
Integrating Machine Learning for Alloy Exploration
J. Foley, Y. Fan, Y. Zhong
Worcester Polytechnic Institute, United States of America

P1.9
Reconstruction of a Historical Silicon Arc-Furnace Thermodynamic Model Using SimuSage and FactFlow
K. Hack, G. Eriksson, K. Poëti, K. Oishi, J-P. Harvey
RWTH Aachen, Germany

P1.10

Microstructure Prediction of Ni–Cr–Al Alloys for Exhaust Valve Spindles Based on Thermodynamic Calculations

H.-S. Jang, J. G. Kim, Y.-y. Woo, E. Y. Yoon
Korea Institute of Materials Science, Korea (Republic of)

P1.11

Nickel Partitioning in Iron and Its Implications for Terrestrial Planet Cores

T. Kovačević, L.X. Benedict, P. Myint, S. Hamel, B. Buffett, B. Militzer
University of California Berkeley, United States of America

P1.12

Stacking Fault Energy in Fe–Mn Steels: Bridging the Gaps between DFT, Experiments and Thermodynamic Modelling

F. Larsson, Y. Mishchenko, Q. Chen, M. Selleby
KTH Royal Institute of Technology, Sweden

P1.13

Experimental Phase Equilibrium Study and Thermodynamic Optimization of the PbO-Na2O-SiO2 System

X. Ling, H. Abdeyazdan, M. Shevchenko, E. Jak, E. Moosavi-Khoonsari, M. Barati
University of Toronto, Canada

P1.14

Experimental Phase Equilibria and Thermodynamic Modeling of the Si3N4-MgO-SiO2 System

C. Luo, B. Yan, T. Deng
Wuhan University of Technology, China

P1.15

Investigation of Additions on β-AlFeSi and α-Hexagonal Phase Formation

V. Rioux-Frenette
Polytechnique Montréal, Canada

P1.16

AI-Driven High-Throughput Design and Performance Iterative Optimization of High Entropy Alloy for Additive Manufacturing

Y. Hou, X. Li, Y. Song, Z. Bi
Research Institute of Advanced Materials CISRI (Shenzhen) Co., Ltd., China

P1.17

Integrated CALPHAD–DFT Study of the Al–Si Subsystem for Accurate Modeling of Si-Containing Steels

Y. Mishchenko, F. Larsson, A. Forslund, Q. Chen, M. Selleby
Royal Institute of Technology, Sweden

P1.18

Construction of Theoretical Phase Diagrams using NNP

H. Okabe, T. Suzuki, M. Enoki, H. Ohtani
JX Advanced Metals Corporation, Japan

P1.19

Microstructural modifications of a 6061 aluminum alloy by addition of iron and vanadium

A. Pomerleau, K. Oishi, M. Brochu, J.-P. Harvey
Polytechnique Montréal, Canada

P1.20

CALPHAD-Based Thermodynamic Framework for Disordered and Ordered Early-Stage Phases in Al alloys

E. Povoden-Karadeniz, E. Kozeschnik
Institute of Materials Science and Technology, Austria

P1.21

From Quantum-Informed Descriptors to Additive Manufacturing Process: A Scale-Bridging Workflow for TCP Phase Prediction

S. Rangaswamy, E. Kabliman
University of Bremen, Germany

P1.22

Advances in the experimental determination of the liquidus projection of the Al-Nb-Ta system

C.S. Barros, J.V. Luiz, C.A. Nunes, G.C. Coelho
University of São Paulo, Brazil

P1.23

Homogenization Kinetics of Refractory High-Entropy Alloys Predicted by Multicomponent Diffusion and DICTRA Simulations

B. Tak, D. Li, M. Ahn, W. Xiong
University of Pittsburgh, United States of America

P1.24

Revisit the Ab Initio Lattice Stability of Cr with R2SCAN Exchange Correlation Function

S. Yang, Y. Zhong
Worcester Polytechnic Institute, United States of America

P1.25

Improving Alloy Mechanical Property Prediction by Addressing Data Homogeneity through Noise Augmentation

Y. Zhang, D. Qiao
Xiamen University of Technology, China

P1.26

Thermodynamic modeling of the Ge-Al-Mg and Ag-Al-Mg systems

A. T. Phan and P. Chartrand
Polytechnique Montréal, Canada

P1.27

Thermodynamic Modeling of Titanium-based Ti-Al-Ca-O Liquid Alloy by Modified Quasichemical Model

G. Hils, M.-K. Paek
Clausthal University of Technology, Germany

Tuesday

Poster Session #2 - June 9, 19:30-21:00, Room 308/309AB

P2.1
Unexpected interfacial reactions in Co/GeTe and Ni/GeTe couples
C.-H. Ho, Y. Chen, S.-W. Chen
National Tsing Hua University, Taiwan

P2.2
Experimental Investigation of Phase Equilibria in Ni-Ce-Cr system
S. M. Dikonda, G. K, H. Tripathy, S. C, M. Vaidya
Indian Institute of Technology Hyderabad

P2.3
Diffusivities and atomic mobilities of fcc phase in Co-rich Co–Fe–Ti system: Experimental study and CALPHAD assessment
J. Sun, D. Ye, Z. Du
University of Science and Technology Beijing, China

P2.4
Thermodynamic modelling of battery cathode materials: early-stage results and perspectives
L. Fenocchio, B. Kaplan, R. L. Jurado, H. Mao, R. Naraghi, M. Selleby
Thermo-Calc Software AB, Sweden

P2.5
Thermodynamic modeling of the Hf-Nb-V system
T. G. Oliveira, A. A. A. P. Silva
Federal University of Itajuba, Brazil

P2.6
Study on microstructure and property of novel γ'-strengthened multi-component Co-based superalloys
F. Chen, Z. Du, D. Wei, J. Shi, C. Guo
University of Science and Technology Beijing, China

P2.7
Bayesian Active Learning of Zero-Phase-Fraction Lines
C. Hardcastle, B. Vela, R. Arróyave
Texas A&M University, United States of America

P2.8
A robotic calorimetry laboratory for phase diagrams on demand
K. Huang, J. Willwerth, A. Rauf, S. Tan, W. Sun
University of Michigan Ann Arbor, United States of America

P2.9
Thermodynamic investigations on the enthalpy of mixing of tributyl phosphate with nitric acid and gadolinium nitrate by micro reaction calorimetry
G. J. Rao, T. Prathibha, S. Balakrishnan, N. Ramanathan, C.V.S. B. Rao, R. Ganesan, V. Jayaraman
HOMI BHABHA NATIONAL INSTITUTE, India

P2.10

The top Calphad scientists according to their citation records

G. Kaptay
University of Miskolc, Hungary

P2.11

Assessment of the Thermodynamics and Thermophysical Properties of the Binary Ag-Pd System

Z. Liang, U. R. Kattner
National Institute of Standards and Technology, United States of America

P2.12

The experimental and theoretical study of the In-La-Ni system

A. Kroupa, R. Žižka, B. Smetana, O. Zobač
Institute of Physics of Materials, Czechia

P2.13

Comparison of model of hydrogen permeation through iron plates with analytical solutions & practical assessment

J.R. Leeman, N. Warnken
University of Birmingham, United Kingdom

P2.14

Modeling and experimental study of IMC formation at Sn/Cu interface

T. Peričková, R. Čička, P. Danišovičová, T. Tánczos
Slovak University of Technology in Bratislava, Slovakia

P2.15

Efficient Single-Phase Region Search via Gradient-Informed Gaussian Processes

C. Maguire, C. Kunselman, B. Vela, R. Arroyave
Texas A&M, United States of America

P2.16

Machine Learning–Accelerated Investigation of Phase Stability in TiVCrCoZr High-Entropy Alloys for Hydrogen Storage Applications

M. Palumbo, G. Pollini, E. M. Dematteis
University of Torino, Italy

P2.17

Thermodynamically Driven Microstructural Evolution and Property Regulation in the Process of Al-Mg-Si Alloys

P. Zhou, M. Yang, Y. Liu, Y. Du
Central South University, China

P2.18

Breaking the Charge Neutrality Boundary in Perovskite Using the PyCALPHAD Approach

A. Shenk, E. Cummings, S. J. Krimmel, R. Otis, Y. Zhong
Worcester Polytechnic Institute, United States of America

P2.19

Liquidus projection of the Co-Si-B system in the Co-rich region

E. K. S. Pellegrino, S. B. V. Boas, A. A. A. P. d. Silva, L. M. Ferreira, M. I. S. T. Faria, G. C. Coelho, C. A. Nunes
University of São Paulo, Brazil

P2.20

Topologically Constrained Machine Learning of Phase Diagrams Using Markov Random Fields

J. Teerman, B. Vela, C. Kunselman, R. Arróyave
Texas A&M University, United States of America

P2.21

Phase equilibria and thermodynamic activities for Li-ion battery electrolytes comprised of LiPF6 in ethylene carbonate and LiPF6 in dimethyl carbonate

M. Trabelsi, H. Al-Salih, Y. A.-L. J.Self
Polytechnique Montréal, Canada

P2.22

Phase diagrams and interfacial reactions of Ni-Bi-Sb ternary system

Y.-H. Lin, Y.-C. Tsai, C.-H. Ho, S.-w. Chen
National Tsing Hua University, Taiwan

P2.23

Physically-constrained prediction of the liquidus curve for multicomponent chemistries

J. Willwerth, S. Tan, A. Rauf, W. Sun
University of Michigan, United States of America

P2.24

Illuminating early-stage oxidation of ZrC using Small-Cell DFT MD

P. Wurzner, Q.-J. Hong, Y. Tang
Technische Universiteit Delft, Netherlands

P2.25

Intelligent Design and Development of Ultra-High-Strength Steels for Additive Manufacturing

X. Li, Y. Hou, Z. Bi
Research Institute of Advanced Materials, China

P2.26

Simulating natural gas substitution by hydrogen with process integration in DRI-MIDREX Process using a novel kinetic approach and equilibrium reactors

U. Mahue, C. Rincent, M. Dubé, G. Laforest, É. Bernier, M. Aghabaranejad, J-P. Harvey
Natural Resources Canada, CanmetENERGY in Varennes, Qc, J3X 1P7, Canada

Author Index

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