CALPHAD

52nd International Conference on Computer Coupling of Phase Diagrams and Thermochemistry

May 25th – 30th, 2025

Paradise Busan Hotel, Busan, Korea

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Hosted by

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Preface

We are pleased to extend a warm welcome to you for the CALPHAD 2025 Conference, which will be held in the dynamic and historically rich city of Busan, South Korea. This prestigious annual event serves as an essential platform for researchers, scientists, and engineers worldwide who are advancing the frontiers of computational thermodynamics and phase diagram modeling.

Since its inception, CALPHAD has been instrumental in shaping our understanding of complex materials systems through thermodynamic modeling and database development. In an era where materials innovation is accelerating across sectors—from energy to aerospace, electronics to sustainable manufacturing—the CALPHAD methodology continues to be a cornerstone in guiding the design and optimization of materials with precision and efficiency. The CALPHAD 2025 conference aspires to deepen these discussions, foster new collaborations, and ignite ideas that will drive the next wave of progress in materials science.

This year, we are proud to host a diverse and distinguished lineup of invited speakers, a single session of technical presentations, and poster presentations, covering a wide range of emerging topics. The participation of leading experts as well as early-career researchers reflects the vibrant and evolving nature of our community. We are also pleased to provide opportunities for interdisciplinary dialogue, as the challenges we face increasingly demand integrated approaches that span beyond traditional boundaries.

We are deeply grateful for the enthusiastic contributions of all presenters, attendees, sponsors, and volunteers whose efforts have made this conference possible. Your presence and engagement are what make CALPHAD 2025 not just an academic event, but a thriving community experience. We would also like to express our heartfelt appreciation to the organizing committee, whose dedication and meticulous planning have brought this vision to life.

As we embark on a week of knowledge-sharing and meaningful exchange, we encourage each of you to take full advantage of the sessions, discussions, and networking opportunities. We shall persist in advancing our discipline through a commitment to curiosity, rigor, and collaboration.

We wish you a fruitful and inspiring conference experience in Busan.

Warm regards,

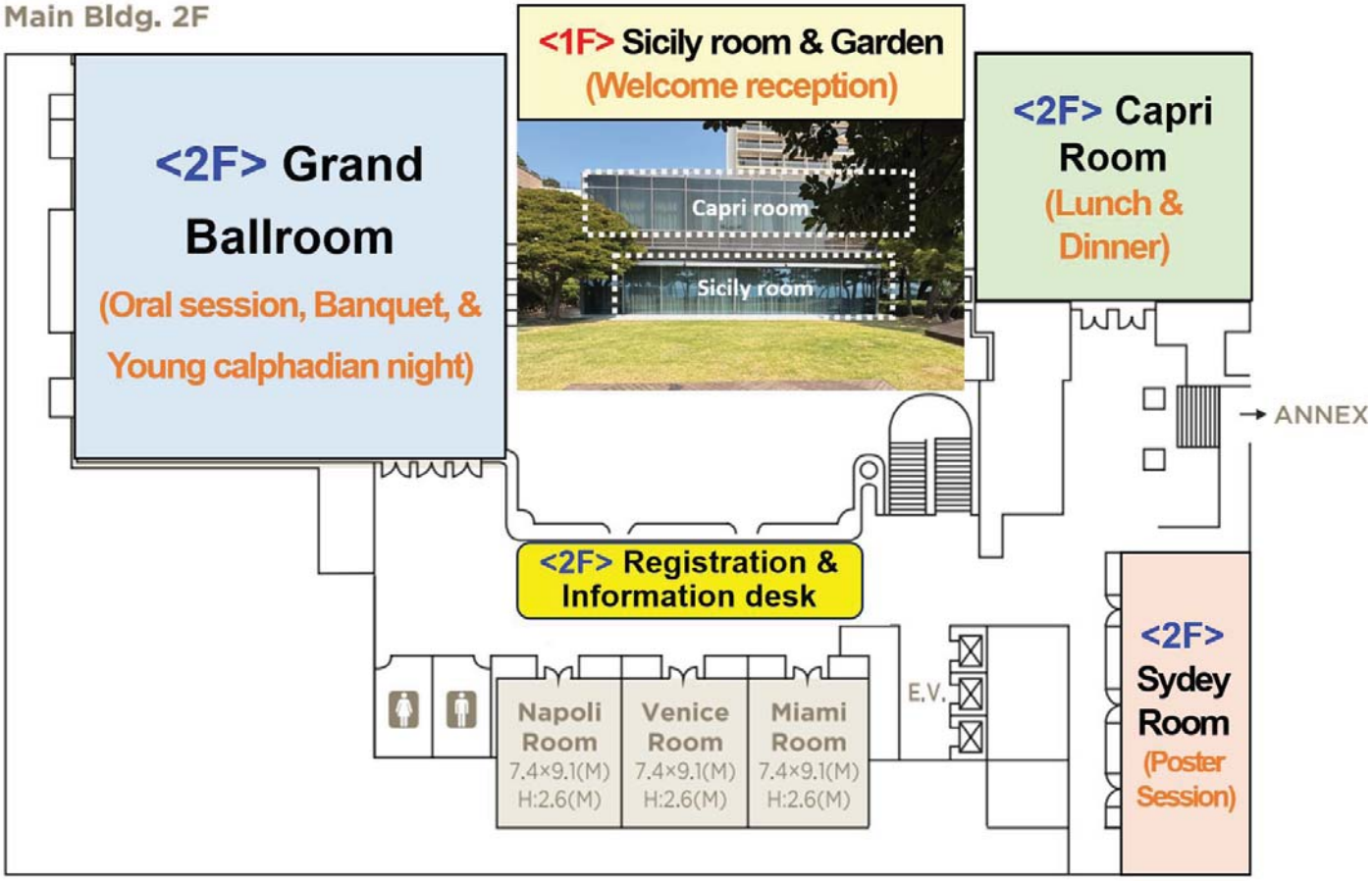
Joonho Lee and Youn-Bae Kang

On the behalf of CALPHAD 2025 organization committee

Program at a Glance

May 25 (SUN)									
<2F> Grand Ballroom / <1F> Sicily Room / <2F> Capri Room / <2F> Sydney Room / External location					Pre-Conference Workshop 13:00–17:00 <Location: Pukyong National University, DAYEON CAMPUS> FactSage, Pandat, PyCalphad, and ThermoCalc			Welcome reception 18:30–19:00 <1F> Sicily room & Garden *Only Snacks & Beverages will be provided.*	
					Registration 16:00–19:00 <2F> Desk located opposite the Venice Room				
May 26 (MON)									
MonIN	MonOR1		MonOR2		MonOR3		MonOR4		MonPO1
08:00–08:50	08:50–10:10	10:10–10:30	10:30–12:10	12:10–14:00	14:00–15:40	15:40–16:10	16:10–18:10	18:10–19:30	19:30–21:00
Invited (1) Prof. Byeong-Joo Lee	Thermodynamic modeling and CALPHAD Assessment (1)	Break (Poster Set-up)	Thermodynamic modeling and CALPHAD Assessment (2)	Lunch (Poster Set-up)	Applications to materials design and process optimization (1)	Break	Experiments for Phase diagram and Thermodynamic property (1)	Dinner	Poster session (1) <2F>Sydey Room
May 27 (TUE)									
TueIN	TueOR1		TueOR2		TueOR3		TueOR4		TuePO1
08:00–08:40	08:40–10:00	10:00–10:20	10:20–12:20	12:20–14:00	14:00–15:40	15:40–16:10	16:10–18:10	18:10–19:30	19:30–21:00
Invited (2) Dr. Cheol-Hee Park	Artificial intelligence - assisted CALPHAD and application (1)	Break (Poster Set-up)	Ab-initio (first-principles) predictions (1)	Lunch (Poster Set-up)	Software development (1)	Break	Software development (2)	Dinner	Poster session (2) <2F>Sydey Room
May 28 (WED)									
WedIN	WedOR1		WedOR2		Excursion				
08:00–08:40	08:40–10:00	10:00–10:20	10:20–12:20	12:20–14:00	14:40–19:00				19:30–22:00
Invited (3) Prof. Yong Jung Kim	Applications to materials design and process optimization (2)	Break	Applications to materials design and process optimization (3)	Lunch	Excursion (Haedong Yonggungsa Temple & Ahopsan Forest Tracking) <Group Bus tour> & Dinner <External restaurants>				Young Calphadian Night <2F> Grand Ballroom
May 29 (THU)									
ThuIN	ThuOR1		ThuOR2		ThuOR3		ThuOR4		
08:00–08:40	08:40–10:00	10:00–10:20	10:20–12:20	12:20–14:00	14:00–15:40	15:40–16:00	16:00–18:00	19:00–21:00	
Invited (4) Prof. Rodney Ruoff	Applications to materials design and process optimization (4)	Break	Diffusion modeling	Lunch	Thermodynamic modeling and CALPHAD Assessment (3)	Break	Experiments for Phase diagram and Thermodynamic property (2)	Banquet (Award announcement) <2F> Grand Ballroom	
May 30 (FRI)									
FriIN	FriOR1		FriOR2						
08:00–08:40	08:40–10:00	10:00–10:20	10:20–12:10	12:10–14:00					
Invited (5) Prof. YongJoo Kim	Ab-initio (first-principles) predictions (2)	Break	Artificial Intelligence - assisted CALPHAD and application (2)	Lunch					

Floor map


Main Bldg. 2F
<2F> Grand Ballroom
(Oral session, Banquet, & Young calphadian night)
<1F> Sicily room & Garden
(Welcome reception)
Capri room
Sicily room
<2F> Capri Room
(Lunch & Dinner)
ANNEX
<2F> Registration & Information desk
Napoli Room
7.4×9.1(M)
H:2.6(M)
Venice Room
7.4×9.1(M)
H:2.6(M)
Miami Room
7.4×9.1(M)
H:2.6(M)
E.V.
<2F> Sydey Room
(Poster Session)

Pre-Conference Workshop

Optional pre-conference workshops will take place on Sunday, May 25 from 13:00 – 17:00 at the Pukyong National University, DAYEON CAMPUS.

Location of pre-conference workshops

Pukyong National University, DAYEON CAMPUS (https://www.pknu.ac.kr/eng/45)
Address: (48513) 45, Yongso-ro, Nam-Gu, Busan, Korea
Bldg. and Room: A15. Hyangpa Bldg. and E22. Dongwon Jang Bogo Hall
FactSage: A15. Hyangpa Bldg. Room 109 (Max. 30 persons)
Pandat: A15. Hyangpa Bldg. Room 209 (Max. 30 persons)
PyCalphad: A15. Hyangpa Bldg. Room 309 (Max. 30 persons)
ThermoCalc: E22. Dongwon Jang Bogo Hall Room 109 (Max. 30 persons)

Direcion Guide:

Kyungsung University–Pukyong National University Station to Pukyong National University Daeyeon Campus Main Gate

This guide provides step-by-step walking directions from Kyungsung University–Pukyong National University Station (Busan Metro Line 2) to the main gate of Pukyong National University's Daeyeon Campus. The route takes approximately 8–10 minutes (600–800 meters).

1. **Exit the Station via Exit 3**
   After arriving at Kyungsung University–Pukyong National University Stationon Busan Metro Line 2, follow signs to Exit 3. This exit is closest to Pukyong National University and leads directly to Suyeong-ro, a main road near the campus.
2. **Turn Left onto Suyeong-ro to Yongso-ro**
   Upon exiting through Exit 3, you'll be on Suyeong-ro. After turning around and short walk, you will find an intersection of Suyeong-ro and Yongso-ro. Then turn left and follow Yongso-ro.
3. **Continue Straight Toward Yongso-ro**
   Walk straight for little more than 400 meters along Yongso-ro. Sooner or later, you'll notice the area becoming more campus-oriented, with fewer commercial buildings.
   After a short more walk along the campus, you'll see the main gate of Pukyong National University's Daeyeon Campus on your left.

4. **Arrive at the Main Gate**
   The gate is prominent, often marked with university signage and a welcoming entrance. The campus address is 45 Yongso-ro, Nam-gu, Busan, and the main gate is easily identifiable.
   The staffs will welcome and guide you there.

Useful links

Google map
Kyungsung Univ- Pukyung Univ Station

Google map
Pukyung Univ. Main gate

Pukyung Univ Hyangpa Bldg., A15

Pukyung Univ
Dongwon Jang Bogo Hall, E22

Pukyung Univ
Campus direction

Pukyung Univ
Virtual map

Social Activities

Excursion: Haedong Yonggungsa Temple & Ahopsan Forest Tracking

Date: May 28th, Wednesday
Cost: Free

Starting Point: Paradise Hotel Busan
Destination: Haedong Yonggugsa Temple & Ahopsan Forest Tracking

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2:00 PM –Departure

- **Starting Point**: Paradise Hotel Busan
- Private vehicle transfer to **Haedong Yonggungsa Temple** (~30 minutes).

2:30 PM – Visit Haedong Yonggungsa Temple

- **Location**: A stunning seaside Buddhist temple.
- Activities:
    - Walk through the temple grounds and admire the scenic ocean views.
    - Explore the temple's iconic landmarks, including the 108 steps, stone pagodas, and the large Buddha statue.
    - Enjoy the serene atmosphere and learn about the temple's history and significance.

3:15 PM – Transfer to Ahopsan Forest

- Drive from Haedong Yonggungsa to **Ahopsan Forest** (~30 minutes).

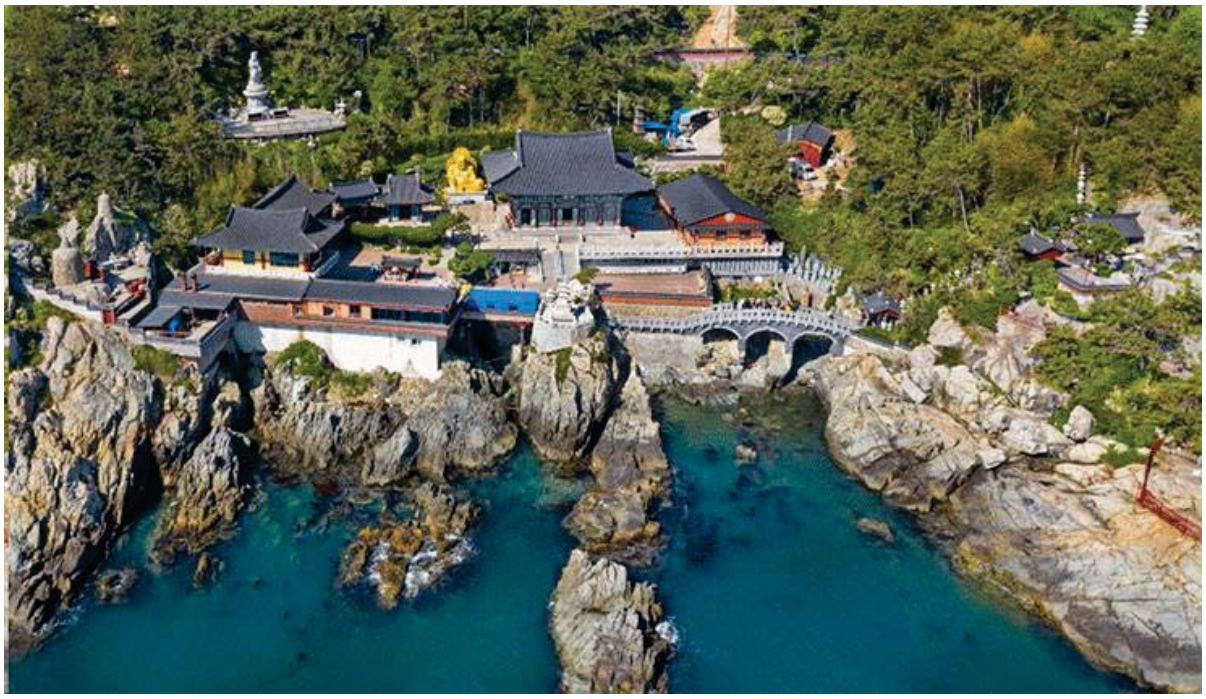
3:45 PM – Ahopsan Forest Trekking

- **Location**: A peaceful bamboo forest known for its natural beauty and tranquility.
- Activities:
    - Guided trekking experience through the lush forest trails (~2 hours).

- Highlights:
    - Bamboo groves, traditional stone walls, and pristine nature.
    - Relaxation activities such as **forest bathing** and mindfulness moments.
- Optional: Participate in **barefoot walking** or light stretching exercises.

5:00 PM – Return to Dinner Restaurant

- Charter bus back to the hotel (~40 minutes).



6:00 PM – Return to Paradise Hotel Busan

Accompanying person tour I: Osiria Coastal Walkway Tracking

Date: May 26th, Monday
Cost: Free

Starting Point: Paradise Hotel Busan
Destination: Osiria Coastal Walkway

9:00 AM – Departure

- Location: Paradise Hotel Busan
- Travel to the Osiria Coastal Walkway by bus (~20 minutes).

9:30 AM – Start Trekking

- Location: Entrance of Osiria Coastal Walkway.
- Activities:
    - Warm-up and stretching (10 minutes).
    - Begin the first section of trekking (~1.5 hours).
    - Enjoy the scenic coastline, ocean breeze, and peaceful atmosphere.

- Highlights: Rocky coastline, wooden observation decks, and lush greenery.

11:00 AM – Midway Break

- Location: Coastal rest area along the path.
- Activities:
  - Take a break for snacks and hydration (15 minutes).
  - Capture photos of the breathtaking ocean views.

11:30 AM – Resume Trekking and Lunch

- Continue walking the final section of the trail (~30 minutes).
- Arrive at the endpoint of the trekking route.
- Have Lunch ((~1 hour)
- Travel back to Paradise Hotel Busan (~20 minutes).

Accompanying person tour II: Songdo Cable Car & Gamcheon Culture Village

Date: May 27th, Tuesday
Cost: Cable car costs will be charged

Starting Point: Paradise Hotel Busan
Destination: Songdo Cable Car & Gamcheon Culture Village

9:00 AM – Departure

- **Starting Point**: Paradise Hotel Busan
- Travel by car to Songdo Sky Park (~30 minutes).

9:30 AM – Songdo Sky Park and Cable Car Experience

- **Location**: Songdo Sky Park
- Activities:

- Ride the **Songdo Marine Cable Car** (round trip, ~20 minutes per ride).
- Enjoy panoramic views of Songdo Beach and the coastline.
- Take photos at the observation deck and explore the Sky Park.

10:30 AM – Gamcheon Culture Village

- **Travel**: Drive from Songdo Sky Park to Gamcheon Culture Village (~15 minutes).
- **Activities**:
  - Stroll through the colorful village famous for its art installations and narrow alleyways.
  - Visit key attractions like the Little Prince Statue and community art murals.
  - Enjoy free time for shopping at local stores or trying light snacks.

11:30 AM – Have Lunch and Return to Paradise Hotel Busan

- Have Lunch (Restaurant)
- **Travel**: Drive back to the hotel (~30 minutes).
- **Wrap-Up**: End of the program; enjoy the rest of the day at your leisure.

Accompanying person tour III: Jagalchi Market & Gukje/Kkangtong Market

Date: May 29th, Thursday
Starting Point: Paradise Hotel Busan
Destination: Jagalchi Market & Gukje/Kkangtong Market

9:00 AM – Departure

- **Starting Point**: Paradise Hotel Busan
- Private vehicle transfer to **Jagalchi Market** (~20 minutes).

9:30 AM – Explore Jagalchi Market

- **Location**: Busan's largest seafood market.
- Activities:
    - Stroll through the bustling stalls selling fresh fish, shellfish, and live seafood.

    - Learn about Korea's seafood culture with a brief introduction by the guide.
    - Optional: Watch or participate in a seafood selection and preparation demonstration.

10:15 AM – Visit Gukje and Kkangtong Market (Connected Areas)

- **Travel**: Short walk (~5 minutes) from Jagalchi Market to Gukje Market.
- Activities:
    - Explore the **Gukje Market**, known for its variety of goods, from souvenirs to local delicacies.
    - Visit the **Kkangtong Market** (Tin Can Market), famous for vintage items and its international market history.
    - Enjoy free time for browsing, shopping, or trying light snacks such as **hotteok (sweet pancakes)** or Korean fried dumplings.

11:30 AM – Lunch at a Local Restaurant

- **Location**: Near Gukje Market or Jagalchi Market.
- Options:
    - Fresh seafood meal at a local restaurant specializing in grilled fish or raw fish platters (hwe).
    - Alternatively, enjoy a variety of Korean dishes, including bibimbap or Korean barbecue, depending on group preferences.

12:30 PM – Return to Paradise Hotel Busan

- Private vehicle transfer back to the hotel (~20 minutes).

Young Calphadian Night 2025

Young Calphadian Night is a traditional evening social event held during the annual CALPHAD conference. All attendees with a young mind are warmly invited to participate and connect with fellow CALPHAD enthusiasts.

The evening will feature **(1) a CALPHAD panel discussion** and **(2) breakout sessions**, where attendees can gain insights into the history of CALPHAD, personal experiences from leading researchers, memorable research stories, and advice on career development in the field.
Drinks will be provided.

1. Plenary panel discussion (1 hour): Moderated by Richard Otis, this session will feature three panelists discussing career paths, research, and perspectives in the CALPHAD community.

2. Breakout sessions (1.5+ hour): Informal small-group discussions (approximately ten people each) that include a mix of local, senior, and young Calphadians. Each group will head to nearby restaurants or bars to continue discussions on CALPHAD careers and enjoy the local culture.

Time
Wednesday, May 28, 2025
7:30 – 10:00 PM
Following the conference excursion.

Location
Paradise Hotel Busan
<2F> Grand Ballroom

Organizers

- Wei Xiong, University of Pittsburgh

- Richard Otis, Proteus Space
- Qi-Jun Hong, Arizona State University
- Zhangting He, Swerim AB
- Florian Tang, GTT Technologies

🎤 Panelists

- Byeong-Joo Lee, Pohang University of Science and Technology
- Afina Lupulescu, FINA Consulting Materials Science and Geology R&D
- Wei Xiong, University of Pittsburgh

🏅 Information about the CALPHAD Young Leader Award

- CALPHAD Awards Page
- CYLA Bylaws PDF (2023)

Oral Presentations

MonIN - Invited (1)

May 26 (Mon), 08:00-08:50, Grand Ballroom

Session Chair: In-Ho Jung (Seoul National University)

MonIN-1 P00074 (08:00 ~ 08:50) **[Invited] CALPHAD: Past, Present and Future**

Byeong-Joo Lee (POSTECH (Pohang University of Science and Technology))*

MonOR1 - Thermodynamic modeling and CALPHAD Assessment (1)

May 26 (Mon), 08:50-10:10, Grand Ballroom

Session Chair: Jae-Hyeok Shim (Korea Institute of Science and Technology)
Sergey Ushakov (Arizona State University)

MonOR1-1 P00050 (08:50 ~ 09:10) **Implications of revising some unaries and binaries in a 31-component database**

Rainer Schmid-Fetzer (Clausthal University of Technology)*

MonOR1-2 P00100 (09:10 ~ 09:30) **Simple relation from interatomic interactions to phase diagram perturbation**

Thomas Hammerschmidt (Ruhr University Bochum), Sarath Menon (Max-Planck-Institute for Sustainable Materials), Ralf Drautz (Ruhr University Bochum)*

MonOR1-3 P00197 (09:30 ~ 09:50) **Key phase diagram experiments and Thermodynamic modeling of the NaCl-KCl-UCl_3 system for Molten Salt Reactor applications**

Taehyoung Kim (Seoul National University), Han Lim Cha, Tae-Hyeong Kim, and Jong-Yun Kim (Korea Atomic Energy Research Institute), In-Ho Jung (Seoul National University)*

MonOR1-4 P00046 (09:50 ~ 10:10) **Modeling non-linear temperature dependence of thermal expansion coefficient in Ni-based superalloys**

Chunan Li (KTH Royal Institute of Technology), David Linder (QuesTek Europe AB), Prajina Bhattacharya (GKN Aerospace), Greta Lindwall (KTH Royal Institute of Technology)*

MonOR2 - Thermodynamic modeling and CALPHAD Assessment (2)

May 26 (Mon), 10:30-12:10, Grand Ballroom

Session Chair: Kateryna Khanchych (KIT)

Patrice Chartrand (Polytechnique Montreal)

MonOR2-1 P00170 (10:30 ~ 10:50) **Common problems in binary assessments**

Bengt Hallstedt (RWTH Aachen University)*

MonOR2-2 P00021 (10:50 ~ 11:10) **Thermodynamic calculation of the Mn-Sb system under external magnetic fields**

Yuchao Shi and Yong Du (Central South University)*

MonOR2-3 P00024 (11:10 ~ 11:30) **Thermodynamic modeling of RE-Te (RE: Ce, Pr, and Nd) systems to mitigate fuel-clad chemical interactions in metallic nuclear fuels**

Soumya Sridar (Indian Institute of Technology Kanpur), Shyam Kumar and Rajesh Ganesan (Indira Gandhi Centre for Atomic Research)*

MonOR2-4 P00045 (11:30 ~ 11:50) **Investigation on the metal-oxide part of the U-Ce-O phase diagram at high temperature**

Caroline Denier, Marc Barrachin, and Bénédicte Michel (ASNR), Luka Vlahovic (European Commission, Joint Research Centre (JRC))*

MonOR2-5 P00141 (11:50 ~ 12:10) **Thermodynamic Modeling of the Ni-Co-Fe-C system**

Min-Kyu Paek (Clausthal University of Technology), Joohyun Park (Hanyang University), In-Ho Jung (Seoul National University)*

MonOR3 - Applications to materials design and process optimization (1)

May 26 (Mon), 14:00-15:40, Grand Ballroom

Session Chair: DongEung Kim (Korea Institute of Industrial Technology)
Denis Shishin (University Of Queensland)

MonOR3-1 P00062 (14:00 ~ 14:20) **A CALPHAD-based Model for Metal Vaporization Prediction in Additive Manufacturing**

Soumya Sridar (Indian Institute of Technology Kanpur), Marcia Myung Hye Ahn and Wei Xiong (University of Pittsburgh)*

MonOR3-2 P00069 (14:20 ~ 14:40) **Integrated Computational Materials Engineering of Fire-Resistant Steels**

Kyoungdoc Kim (Pohang University of Science and Technology)*

MonOR3-3 P00106 (14:40 ~ 15:00) **CALPHAD-assisted design of high-performance TiAl alloys and special refractory materials**

Qisheng Feng (shanghai university), Rong Shi, Linjun Wang, and Chonghe Li (Shanghai University)*

MonOR3-4 P00157 (15:00 ~ 15:20) **Recent Progress of Solution Model for Predicting the Properties of Multicomponent Systems**

Jun Luan, Zhigang Yu, and Kuochih Chou (Shanghai University)*

MonOR3-5 P00115 (15:20 ~ 15:40) **Thermodynamic Desing Framework Applied to In Situ Nb(N,C)-Reinforced Ferrous Matrix Composites**

Isadora Schramm Deschamps, Eduardo Moraes Souza, Fernando Miyata, and Aloisio Nelmo Klein (Federal Univesity of Santa Catarina)*

MonOR4 - Experiments for Phase diagram and Thermodynamic property (1)

May 26 (Mon), 16:10-18:10, Grand Ballroom

Session Chair: In-Ho Jung (Seoul National University)
Viera Homolova (Institute of Materials Research, Slovak Academy of Sciences)

MonOR4-1 P00018 (16:10 ~ 16:30) **Directional solidification of Sn-Bi-Cu and Sn-Cu-Sb alloys**

Sinn-wen Chen, Hsin-Chieh Huang, and Yen-Yi Chen (National Tsing Hua University)*

MonOR4-2 P00031 (16:30 ~ 16:50) **Phase Diagram of Janus-type Bi–Sn Alloy Nanoparticles**

Joonho LEE and Hangyeol Kim (Korea University), Guy Makov (Ben-Gurion University of the Negev)*

MonOR4-3 P00151 (16:50 ~ 17:10) **Some practical aspects on modeling evolution of precipitates in casting and thermomechanical processing of steels**

Chunhui Luo, Erik Claesson, and Hans Magnusson (Swerim AB)*

MonOR4-4 P00079 (17:10 ~ 17:30) **Liquidus projection of the In-Sb-Zn system**

Ondrej Zobac (Institute of Physics of Materials CAS), Przemyslaw Fima (Institute of Metallurgy and Materials Science PAS)*

MonOR4-5 P00108 **Gallium as a Solvent for the Thermodynamic Study of Non-Oxide Materials**

(17:30 ~ 17:50) **Using an MHTC-96 High Temperature Calorimeter**

Michael Bustamante, Manuel Scharrer, Jared Matteucci, and Alexandra Navrotsky (ARIZONA STATE UNIVERSITY)*

MonOR4-6 P00120 (17:50 ~ 18:10) **Study on the effect of alloying element for microstructure control with high performance safty steel using thermodynamic calculation**

JunHo Chung, Jae-chang Song, Chul-won Lee, and Jin-Hyoek Kim (Hyundai Steel Company), Dong-ik Kim (Korea Institute of Science Technology), Bong-ho Lee (Daegu Gyeongbuk Institute of Science and Technology), Hyun-Uk Hong (Changwon National University), Chang-Hoon Lee (Korea Institute of Materials Science)*

TueIN - Invited (2)

May 27 (Tue), 08:00-08:40, Grand Ballroom

Session Chair: In-Ho Jung (Seoul National University)

TueIN-1 P00226 (08:00 ~ 08:40) **[Invited] Open Innovation to Accelerate Technological Development of Batteries**

Cheol-Hee Park (LG Energy Solution)*

TueOR1 - Artificial intelligence - assisted CALPHAD and application (1)

May 27 (Tue), 08:40-10:00, Grand Ballroom

Session Chair: Chuan Zhang (CompuTherm LLC)
Qijun Hong (Arizona State University)

TueOR1-1 P00072 (08:40 ~ 09:00) **Perspectives on CALPHAD in the AI Era**

Zi-Kui Liu (PENN STATE UNIV)*

TueOR1-2 P00089 (09:00 ~ 09:20) **Thermodynamic Modeling of the σ Phase based on Density Functional Theory and Graph Neural Network**

Wenhao Zhang (National Institute for Materials Science), Mariano Forti (Ruhr-University), Runan Xie, Celine Barreteau, and Jean-Marc Joubert (East Paris Institute of Chemistry and Materials), Taichi Abe (National Institute for Materials Science), Thomas Hammerschmidt (Ruhr-University), Jean-Claude Crivello (National Institute for Materials Science)*

TueOR1-3 P00088 (09:20 ~ 09:40) **Pt-Rh Thermodynamic Database using Neural Network Potential**

Arkapol Saengdeejing, Ryoji Sahara, Hiori Kino, and Toyohiro Chikyow*

(National Institute for Materials Science)

TueOR1-4 P00117 (09:40 ~ 10:00) **Screening new Entropy Stabilized Oxides by DFT calculations and active learning**

Sebastien Junier (CNRS, ICMPE, Univ Paris Est Creteil), Celine Barreteau (Univ Paris Est Creteil, CNRS, ICMPE), Christophe Bajan and Guillaume Lambard (NIMS), Jean-Claude Crivello (LINK, CNRS, St. Gobain, NIMS)*

TueOR2 - Ab-initio (first-principles) predictions (1)

May 27 (Tue), 10:20-12:20, Grand Ballroom

Session Chair: Marcel Sluiter (Delft University of Technology)
Won-Seok Ko (Inha University)

TueOR2-1 P00102 (10:20 ~ 10:40) **Atomic (Inter)Diffusion Coefficients in Medium/High Entropy Alloys – First-Principles Combined with Cluster Variation Method**

Chaoping Liang, Haiyu Luo, Guangxiong Luo, Wensheng Liu, and Yunzhu Ma (Central South University)*

TueOR2-2 P00130 (10:40 ~ 11:00) **Automated and computationally efficient computation of fully ab initio binary phase diagrams**

Joerg Neugebauer, Sarath Menon, Marvin Poul, and Tilmann Hickel (Max Planck Institute for Sustainable Materials)*

TueOR2-3 P00131 (11:00 ~ 11:20) **Segregation, ordering and solvent effects at Mg-alloy surfaces with Ca studied by ab initio surface phase diagrams**

Mira Todorova, Jing Yang, Ahmed Abdelkawy, and Joerg Neugebauer (Max Planck Institute for Sustainable Materials)*

TueOR2-4 P00140 (11:20 ~ 11:40) **Revisiting Entropy in FCC Phase of Nb, Mo, and W: Implications for Phase Stability and CALPHAD Modeling**

Qijun Hong (Arizona State University), Qing Chen (Thermo-Calc, KTH)*

TueOR2-5 P00188 (11:40 ~ 12:00) **Integrated Study of First-principles Calculations and Experimental Structure Analysis for Fluorination reaction of CuS positive electrode**

Yongpeng Tang and Soichiro Matsumi (Kyushu University), Kosuke Noi (Kyoto University), Takashi Honda (High Energy Accelerator Research Organization), Hidenori Miki (Toyota Motor Corporation), Satoshi Iikubo (Kyushu University)*

TueOR2-6 P00211 (12:00 ~ 12:20) **Atomistic Modeling and Phase Equilibria of Pt-Noble Metal Binary Alloys: From Bulk to Nanoalloys**

HOSEOK NAM and Kayoung Yun (Kookmin University)*

TueOR3 - Software development (1)

May 27 (Tue), 14:00-15:40, Grand Ballroom

Session Chair: Zhenmin Du (University of Science and Technology Beijing)
Jiwon Park (Korea Institute of Materials Science)

TueOR3-1 P00181 (14:00 ~ 14:20) **A path towards semantically correct and information rich databases**

Florian Tang (GTT Technologies), Brandon Bocklund (Lawrence Livermore National Laboratory), Richard Otis (Proteus Space Inc.), Moritz to Baben (GTT Technologies), Johan Zietsman (Ex Mente Ltd.)*

TueOR3-2 P00189 (14:20 ~ 14:40) **Automatic extraction of datasets and design of amorphous and nanocrystalline alloy with desired properties**

Chengying Tang (Guilin University of Electronic Technology)*

TueOR3-3 P00217 (14:40 ~ 15:00) **FactFlow Process Simulation for Sustainable Metallurgy: Integrating Thermodynamics, LCA, and Optimization**

Kyota Poeti, Kentaro Oishi, Daniel Wei, Eve Bélisle, Patrice Chartrand, and Jean-Philippe Harvey (Polytechnique Montréal)*

TueOR3-4 P00196 (15:00 ~ 15:20) **LACOS: Cluster Expansion Modelling of Complex Multicomponent Alloy Thermodynamics Simplified**

Seung-Cheol Lee (Indo Korea S & T Center, KIST), Krishnamohan Thekkepat (Korea Institute of Science and Technology), Debi Prasad Dogra (Indian Institute of Technology Bhubaneswar)*

TueOR3-5 P00067 (15:20 ~ 15:40) **Non-Local Equilibrium Thermodynamics and Kinetics during Fast Advancement of Transformation Interface**

Kaisheng Wu (Thermo-Calc Software Inc), Qing Chen and Johan Jeppsson (Thermo-Calc Software AB)*

TueOR4 - Software development (2)

May 27 (Tue), 16:10-18:10, Grand Ballroom

Session Chair: Florian Tang (GTT Technologies)

Wei Xiong (University of Pittsburgh)

TueOR4-1 P00008 (16:10 ~ 16:30) **Breaking the Charge Neutrality Boundary in Perovskite Using the PyCALPHAD Approach**

Yu Zhong (Worcester Polytechnic Institute)*

TueOR4-2 P00056 (16:30 ~ 16:50) **Phase Field modeling of L10 ordered phase in Fe-Ni system: from meteorite to permanent magnet**

Helena Zapolsky (CNRS GPM UMR 6634 University of Rouen), Siyuan He, Renaud Patte, and Frederic Danoix (GPM UMR 6634 University of Rouen)*

TueOR4-3 P00068 (16:50 ~ 17:10) **Generating Alloy Thermodynamic and Thermophysical Data Using CALPHAD**

Andre Schneider, Nicholas Grundy, and Hai-Lin Chen (Thermo-Calc Software AB), Kaisheng Wu (Thermo-Calc Sofwtare Inc.), Reza Naraghi and Qing Chen (Thermo-Calc Software AB)*

TueOR4-4 P00070 (17:10 ~ 17:30) **Barycentric Coordinate System**

Shuanglin Chen (CompuTherm, LLC)*

TueOR4-5 P00116 (17:30 ~ 17:50) **Accelerating Alloy Design with TAOS**

Brandon Bocklund (Lawrence Livermore National Laboratory)*

TueOR4-6 P00054 (17:50 ~ 18:10) **Gradient-Based Optimization of CALPHAD Model Parameters**

Courtney Kunselman (Texas A&M University), Brandon Bocklund (Lawrence Livermore National Laboratory), Richard Otis (Proteus Space Inc.), Raymundo Arroyave (Texas A&M University)*

WedIN - Invited (3)

May 28 (Wed), 08:00-08:40, Grand Ballroom

Session Chair: Youn-Bae Kang (POSTECH)

WedIN-1 P00227 (08:00 ~ 08:40) **[Invited] Diffusion Leads to Fractionation Phenomena in a Heterogeneous Environment**

Yong-Jung Kim (Korea Advanced Institute of Science and Technology (KAIST))*

WedOR1 - Applications to materials design and process optimization (2)

May 28 (Wed), 08:40-10:00, Grand Ballroom

Session Chair: Hyo-Sun Jang (Korea Institute Of Materials Science)
Andre Schneider (Thermo-Calc Software AB)

WedOR1-1 P00152 (08:40 ~ 09:00) **Nd Speciation during Electrowinning in Molten Chlorides**

Nicholas Ury, Brandon Bocklund, and Emily Moore (Lawrence Livermore National Laboratory), Ben Holcombe and Rohan Akolkar (Case Western Reserve University), Aurelien Perron (Lawrence Livermore National Laboratory)*

WedOR1-2 P00160 (09:00 ~ 09:20) **First-principles materials genome approach for solid-state electrolytes: formulation and experimental exploitation**

GUOSHENG SHAO (Zhengzhou University)*

WedOR1-3 P00166 (09:20 ~ 09:40) **Simulation-driven optimization of energy-efficient manufacturing of large steel products**

Zhangting He, Niklas Holländer Pettersson, Pontus Darth, Mattias Ek, Jesper Önell, Nils Andersson, and Stefan Marth (Swerim), Tomas Nordqvist, Mikael Andreasson, and Lars Nordström (Björneborg Steel)*

WedOR1-4 P00193 (09:40 ~ 10:00) **The role of solid solution and particle morphology in iron phosphate-based electrodes for selective electrochemical lithium extraction**

Wei Chen (University at Buffalo)*

WedOR2 - Applications to materials design and process optimization (3)

May 28 (Wed), 10:20-12:20, Grand Ballroom

Session Chair: Jean-Marc Joubert (CNRS)
Jean-Philippe Harvey (Polytechnique Montreal)

WedOR2-1 P00005 (10:20 ~ 10:40) **Entropy as a Predictive Tool for Radiation Intensity and Photoluminescence: A Thermodynamic Approach**

Ping Wu (Singapore University of Technology and Design)*

WedOR2-2 P00042 (10:40 ~ 11:00) **Phase diagram of $BaTiO_3$-$CaTiO_3$ with morphotropic phase boundaries derived by Landau-Devonshire**

Weiping Gong (Huizhou University)*

WedOR2-3 P00051 (11:00 ~ 11:20) **Leveraging CALPHAD modeling for e-waste pyrometallurgical recycling**

Denis Shishin, Maksym Shevchenko, and Evgueni Jak (University Of Queensland)*

WedOR2-4 P00052 (11:20 ~ 11:40) **On the evolution of β1/β′ coupled-structures in Mg–Y–Nd alloys: A simulation study**

Hong Liu and Jing Luo (Shanghai Jiao Tong University), Nele Moelans (KU Leuven), Liming Peng (Shanghai Jiao Tong University), Jian-Feng Nie (Monash University)*

WedOR2-5 P00015 (11:40 ~ 12:00) **The Role of Molybdenum (Mo) and Nickel (Ni) in Tool Steel on Interaction Layer Formation with Molten Aluminum Alloys**

Maja Voncina, Aleš Nagode, Jožef Medved, and Tilen Balaško (University of Ljubljana, Faculty of Natural Science and Engineering)*

WedOR2-6 P00149 (12:00 ~ 12:20) **Improving Weld Oxygen Composition Predictions using Process-Informed CALPHAD Modeling**

Thomas Avey, Dan Bechetti, and Charles Fisher (Naval Surface Warfare Center Carderock)*

ThuIN - Invited (4)

May 29 (Thu), 08:00-08:40, Grand Ballroom

Session Chair: Youn-Bae Kang (POSTECH)

ThuIN-1 P00228 (08:00 ~ 08:40) **[Invited] New Methods to Grow Diamond and Cubic Boron Nitride?**

*Rodney Ruoff * (Ulsan National Institute of Science and Technology (UNIST))*

ThuOR1 - Applications to materials design and process optimization (4)

May 29 (Thu), 08:40-10:00, Grand Ballroom

Session Chair: Yu Zhong (Worcester Polytechnic Institute)
Krishnamohan Thekkepat (Korea Institute of Science and Technology)

ThuOR1-1 P00203 (08:40 ~ 09:00) **Diffusion in Molten Silicate System: Experiments and Model**

Ihnbeom Lee and In-Ho Jung (Seoul National University)*

ThuOR1-2 P00144 **Comparative study of the effects of oxygen potential buffer in chromium-**

(09:00 ~ 09:20) **doped and undoped UO_2 fuel**

Morgane ROCHEDY, Jacques Léchelle, and Chantal Riglet-Martial (CEA)*

ThuOR1-3 P00060 (09:20 ~ 09:40) **CALPHAD Coupled Phase-Field Simulation for Additive Manufacturing of High Entropy Alloys**

Kate Elder and Scott Peters (Lawrence Livermore National Laboratory), Joni Kaipainen (VTT Technical Research Centre of Finland), Saad Khairallah (Lawrence Livermore National Laboratory), Adam Krajewski (The Pennsylvania State University), Brandon Bocklund (Lawrence Livermore National Laboratory), Lassi Linnala and Gizem Isitman (VTT Technical Research Centre of Finland), Hernan Villanueva (Lawrence Livermore National Laboratory), Jean-Luc Fattebert (Oak Ridge National Laboratory), Scott McCall and Joseph McKeown (Lawrence Livermore National Laboratory), Tom Andersson, Anssi Laukkanen, and Tatu Pinomaa (VTT Technical Research Centre of Finland), Aurelien Perron (Lawrence Livermore National Laboratory)*

ThuOR1-4 P00016 (09:40 ~ 10:00) **Thermal stability of Hot-Work Tool Steel alloyed with Ta**

Jozef Medved, Maja Vončina, and Tilen Balaško (University of Ljubljana), Jaka Burja (Institute of Metals and Technology), Klemen Grabnar (Metal Tech Solutions d.o.o.)*

ThuOR2 - Diffusion modeling

May 29 (Thu), 10:20-12:20, Grand Ballroom

Session Chair: Xiaoyu Zheng (Central South University)
Anders Engstrom (Thermo-Calc Software)

ThuOR2-1 P00007 (10:20 ~ 10:40) **CALPHAD Assessments of Mobilities Using Simple Models and Holistic Integration of Experimental & Computed Data**

Ji-Cheng (JC) Zhao (University of Connecticut)*

ThuOR2-2 P00086 (10:40 ~ 11:00) **Quantitative analysis of diffusion equation when diffusivity is givenas function of concentration**

Yeonhak Chu and Kunok Chang (Kyung Hee University)*

ThuOR2-3 P00105 (11:00 ~ 11:20) **CALPHAD-based models for complex diffusion phenomena in compositionally-graded Ni-based superalloys**

Ahmadreza Riyahi khorasgani and Julia Kundin (Ruhr university Bochum), Bettina Camin (Hochschule Bremerhaven, Bremerhaven), Ingo Steinbach (Ruhr university Bochum)*

ThuOR2-4 P00214 (11:20 ~ 11:40) **A new CALPHAD-integrated strategy to deduce atomic mobility for high-entropy alloy system: a case study on fcc Ni-Co-Al-Cr system**

Xue-Ting Wu (Anhui University of Technology), Xiao-Gang Lu (Shanghai University)*

ThuOR2-5 P00221 (11:40 ~ 12:00) **Ab initio thermodynamic-and-kinetic phase diagram to evaluate quasicrystal stability and synthesizability**

Woohyeon Baek, Sambit Das, Shibo Tan, Vikram Gavini, and Wenhao Sun (University of Michigan)*

ThuOR2-6 P00041 (12:00 ~ 12:20) **Generation of mobility database in correlation to various experimental methods and PINN-based numerical inverse method in ternary and Multicomponent system**

Suman Sadhu and Surendra Kumar Makineni (Indian Institute of Science Bengaluru), Saswata Bhattacharya (Indian Institute of Technology Hyderabad), Aloke Paul (Indian Institute of Science Bengaluru)*

ThuOR3 - Thermodynamic modeling and CALPHAD Assessment (3)

May 29 (Thu), 14:00-15:40, Grand Ballroom

Session Chair: Zhangting He (Swerim)
Min-Kyu Paek (Clausthal University of Technology)

ThuOR3-1 P00080 (14:00 ~ 14:20) **Thermodynamic Modeling of Metastable and Transition Carbides in the Fe-C System**

QING CHEN (Thermo-Calc Software AB), Changming Fang (Brunel University London), Reza Naraghi (Thermo-Calc Software AB), Malin Selleby and John Ågren (KTH Royal Institute of Technology)*

ThuOR3-2 P00191 (14:20 ~ 14:40) **An AI-Enhanced Closed-Loop Framework for CALPHAD Optimization of Metastable Phases in Al-Cu-Mg-Si Alloys**

Kai Tang and Qiang Du (SINTEF AS)*

ThuOR3-3 P00134 (14:40 ~ 15:00) **Thermochemistry of neodymium silicates and reassessment of the Nd_2O_3-CaO-SiO_2 system**

Wenjie Wei, Shu Li, and Zhanmin Cao (University of Science & Technology Beijing)*

ThuOR3-4 P00047 (15:00 ~ 15:20) **Evolution of Al-Ti complex oxide inclusions during Ti-added Ultra Low C Steel: Thermodynamic Modeling and Diffusion Analysis**

Young-Joon Park and Youn-Bae Kang (Pohang University of Science and Technology)*

ThuOR3-5 P00098 (15:20 ~ 15:40) **Surface tension calculation of TiO_2-bearing slags**

Buxin Chen, Chenguang Bai, Meilong Hu, Yucen Kuang, and Shengfu Zhang (Chongqing University)*

ThuOR4 - Experiments for Phase diagram and Thermodynamic property (2)

May 29 (Thu), 15:40-17:40, Grand Ballroom

Session Chair: Youngjo Kang (Dong-A University)
Ales Kroupa (Institute of Physics of Materials)

ThuOR4-1 P00110 (15:40 ~ 16:00) **Experimental and theoretical phase equilibria in the system In-La-Ni**

Ondrej Zobac (Institute of Physics of Materials CAS, v.v.i., CZ68081723), Lubomir Kral (IPM CAS, v.v.i.), Bedrich Smetana (VSB-TUO), Ales Kroupa (IPM CAS, v.v.i.)*

ThuOR4-2 P00190 (16:00 ~ 16:20) **Enhancing Energy Storage Materials: New Developments in Thermal Analysis**

Dmitry Sergeev (NETZSCH A&T), Gwilherm Nénert (Malvern Pananalytical B.V.), Doreen Rapp, Fabia Beckstein, and Michael Schöneich (NETZSCH A&T), Michael Müller (Forschungszentrum Juelich), Jan Gertenbach (Malvern Pananalytical B.V.), Jan Hanss (NETZSCH A&T)*

ThuOR4-3 P00065 (16:20 ~ 16:40) **Thermodynamic Evaluation of the $CaCl_2$-CaF_2-$CaSO_4$ System**

Rhys Jacob (Forschungszentrum Juelich), Amedeo Morsa, Elena Yazhenskikh, and Michael Müller (Forschungszentrum Jülich)*

ThuOR4-4 P00104 (16:40 ~ 17:00) **Integrated of experimental phase equilibrium, calorimetric study, and thermodynamic modeling of the MnO-V_2O_5 system**

zhuoyang Li (Chongqing University), Guishang Pei (Seoul National University), Mengjiao Jiao, Yang Zhang, and Xuewei Lv (Chongqing University)*

ThuOR4-5 P00192 (17:00 ~ 17:20) **Thermodynamic Analysis of Phase Equilibria in the Ge-Sn Binary System Considering Particle Size**

Tatsuya Tokunaga, Robin Yoneda, and Asuka Tsuru (Kyushu Institute of Technology)*

ThuOR4-6 P00084 (17:20 ~ 17:40) **CALPHAD-integrated Density-based Thermodynamics of Grain Boundaries**

Reza Darvishi Kamachali (Federal Institute for Materials Research and Testing)*

FriIN - Invited (5)

May 30 (Fri), 08:00-08:40, Grand Ballroom

Session Chair: Yongwoo Kwon (Hongik University)

FriIN-1 P00216 (08:00 ~ 08:40) **[Invited] Active learning-based design of multi-metallic alloy nanocatalyst**

YongJoo Kim (Korea University)*

FriOR1 - Ab-initio (first-principles) predictions (2)

May 30 (Fri), 08:40-10:00, Grand Ballroom

Session Chair: Hoseok Nam (Kookmin University)
Yongwoo Kwon (Hongik University)

FriOR1-1 P00212 (08:40 ~ 09:00) **Modelling tramp elements in steel with fine-tuned machine learned interatomic potential**

Naveen Karuthodi Mohandas and Marcel HF Sluiter (Delft University of Technology)*

FriOR1-2 P00175 (09:00 ~ 09:20) **Accelerating the design of Al-Mg-Zn alloys with limited data via active learning and CALPHAD-based transfer learning**

Wuwei Mo, Yuling Liu, and Yong Du (Central South University)*

FriOR1-3 P00061 (09:20 ~ 09:40) **Full-scale Monte Carlo Potts simulation for practical applications**

Sang-Ho Oh and Byeong-Joo Lee (Pohang University of Science and Technology)*

FriOR1-4 P00164 (09:40 ~ 10:00) **Building a thermodynamic database for compositionally complex transition metal carbides using first-principles calculations and uncertainty quantification guided experiments**

Theresa Davey (Bangor University), William Rosenberg and Scott McCormack (University of California Davis), Ying Chen (Tohoku University)*

FriOR2 - Artificial Intelligence - assisted CALPHAD and application (2)

May 30 (Fri), 10:20-12:10, Grand Ballroom

Session Chair: DongEung Kim (Korea Institute of Industrial Technology)
Sang-Ho Oh (POSTECH)

FriOR2-1 P00103 (10:20 ~ 10:40) **Site occupancies in the most complex TCP phases studied by synchrotron diffraction, DFT and machine learning**

Jean-Marc Joubert and Ahmed Aissaoui (CNRS), Agustin Flores (CEA), Chancel Mawalala-Moundounga (CNRS), Mariano Forti (ICAMS), Wenhao Zhang (LINK), Thomas Hammerschmidt (ICAMS), Jean-Claude Crivello (LINK)*

FriOR2-2 P00058 (10:40 ~ 11:00) **Atomistic simulations of phase stability and deformation behaviors in shape-memory alloys**

Won-Seok Ko (Inha University), Jung Soo Lee (Max Planck Institute for Sustainable Materials), Blazej Grabowski (University of Stuttgart)*

FriOR2-3 P00186 (11:00 ~ 11:20) **Theory-Driven Insights for Advanced Battery Materials**

TAEHUN LEE (Jeonbuk National University)*

FriOR2-4 P00215 (11:20 ~ 11:40) **Compositional Space Graphs as a Novel Approach for Efficient Exploration of High-Dimensional Design Spaces**

Adam M Krajewski (The Pennsylvania State University), Alexander M Richter (Penn State University), Ricardo Amaral (The Pennsylvania State University), Zi-Kui Liu (PENN STATE UNIV)*

FriOR2-5 P00219 (11:40 ~ 12:00) **A Classified Dataset and Hierarchical Iteration Method to Assess M_s Temperatures**

Guanglong Xu, Jinlei Lu, Fuwen Chen, and Yuwen Cui (Nanjing Tech University)*

Poster Presentations

MonPO - Poster session (1)

May 26 (Mon), 19:30-21:00, Sydney Room

Session Chair:

MonPO-1 P00004 (19:30 ~ 21:00) **Thermodynamics and interplay of Al-, B-, and Ti-Nitrides in microalloyed steel.**

Markus Fuehrer (TU Wien, Institut 308), Sabine Zamberger (Voestalpine Forschungsservicegesellschaft), Erwin Povoden-Karadeniz (TU Wien)*

MonPO-2 P00006 (19:30 ~ 21:00) **DFT guided defect engineering in MgO nanostructures for enhanced CO_2 Capture**

*Hashan Nuwantha Thenuwara and Shunnian Wu (Singapore University of Technology and Design), Bella S. (Institute of Sustainability for Chemicals, Energy & Environment, Agency for Science, Technology and), Siew-Yee Wong and Li Xu (Institute of Materials Research and Engineering, Agency for Science, Technology and Research (A*STAR), Ping Wu* (Singapore University of Technology and Design)*

MonPO-3 P00009 (19:30 ~ 21:00) **Experimental Investigations and DICTRA Simulations on Microstructure Evolution of Direct-Quenched Steels during Intercritical Annealing**

Seung-Hyeok Shin, Dong-Kyu Oh, and Byoungchul Hwang (Seoul National University of Science and Technology)*

MonPO-4 P00010 (19:30 ~ 21:00) **Effects of Carbon Vacancy in MC Nano-Precipitates on Hydrogen Embrittlement of Tempered Martensitic Steel**

Sang-Gyu Kim and Byoungchul Hwang (Seoul National University of Science and Technology (SEOULTECH))*

MonPO-5 P00011 (19:30 ~ 21:00) **Liquidus projections and miscibility gaps in theSn-Bi-Cu-Te quaternary system**

Cheng-Hsi Ho, Hsin-Chieh Huang, Yung-Chun Tsai, and Sinn-wen Chen (NATIONAL TSING HUA UNIVERSITY)*

MonPO-6 P00013 (19:30 ~ 21:00) **Bi-Co-Sb phase equilibria and Co/(Bi,Sb) interfacial reactions**

Cheng-Hsi Ho, Hong-Dian Chiang, and Sinn-wen Chen (NATIONAL TSING HUA UNIVERSITY)*

MonPO-7 P00012 (19:30 ~ 21:00) **Liquidus projection and liquid miscibility gaps in Ag-Cu-Se and Cu-Se-Te ternary systems**

Yung-Chun Tsai, Yung-Jen Chuang, and Sinn-wen Chen (NATIONAL TSING HUA UNIVERSITY)*

MonPO-8 P00014 (19:30 ~ 21:00) **Phase equilibria of Co-Ge-Sb system**

Yung-Chun Tsai, Cheng-Hsi Ho, and Sinn-wen Chen (NATIONAL TSING HUA UNIVERSITY)*

MonPO-9 P00017 (19:30 ~ 21:00) **Modeling multicomponent hydrides in para-equilibrium: Software and prediction**

Peter Hannappel, Marcus Vogt, Felix Heubner, Mateusz Balcerzak, and Thomas Weißgärber (Fraunhofer Institution)*

MonPO-10 P00019 (19:30 ~ 21:00) **Decoupling Atomic Diffusion Degeneracy in $L1_2$ Intermetallics**

Haiyu Luo, Wensheng Liu, and Chaoping Liang (Central south university)*

MonPO-11 P00020 (19:30 ~ 21:00) **Diffusivity and atomic mobility assessments of U-Nb and U-Mo melts: a combined AIMD and CALPHAD study**

Hui Yang and Yong Du (Central South University)*

MonPO-12 P00022 (19:30 ~ 21:00) **Experimental and thermodynamic study of microstructure evolution at SAC305-xNi/Cu interface**

Tereza Machajdikova, Roman Čička, Ivona Černíčková, Libor Ďuriška, Marián Drienovský, and Peter Gogola (Slovak University of Technology)*

MonPO-13 P00023 (19:30 ~ 21:00) **Structural and thermal study of the gallium-enriched SAC305 lead-free solders**

Patricia Danisovicova, Ivona Černičková, Libor Ďuriška, and Marián Drienovský (Slovak University of Technology)*

MonPO-14 P00025 (19:30 ~ 21:00) **Crystallization Modeling of Zr and Fe-Based Metallic Glass**

Nils Mattias Tidefelt (Malmo University), Julia Löfstrand, Inga Katharina Goetz, and Olivier Donzel-Gargand (Uppsala University),*

Anders Ericsson (Lund University), Han Xiaoliang (Leibniz Institute for Solid State and Materials Research), Petra Jönsson and Martin Salhberg (Uppsala University), Ivan Kaban (Leibniz Institute for Solid State and Materials Research), Martin Fisk (Malmö University / Lund University)

MonPO-15 P00026 (19:30 ~ 21:00)

Thermodynamic analysis on adsorption of sulfur on liquid Fe-3wt%Si alloy

Jiwoo Park (Korea University), Ji Woong Yu (Korea Institute for Advanced Study), YongJoo Kim and Joonho Lee (Korea University)*

MonPO-16 P00027 (19:30 ~ 21:00)

Isopiestic vapour pressure measurements and thermodynamic modelling of the La-Te system

S Shyam Kumar (HBNI, IGCAR), Sridar Soumya (Indian Institute of Technology Kanpur), Ganesan Rajesh (IGCAR)*

MonPO-17 P00028 (19:30 ~ 21:00)

Impact of Vaporization on Experimental Work: The Case of Molybdate Oxides

Kaoutar Naciri and Ioana Nuta (SIMaP - CNRS), Evelyne Fischer (SIMaP), Guillaume Deffrennes, Alexander Pisch, and Matias Velazquez (SIMaP - CNRS)*

MonPO-18 P00029 (19:30 ~ 21:00)

A discrete number diffusion scheme to model atomic transport behaviour, with an application to nickel oxide.

Harry Ho Yeen Craven, Mary Taylor, and Nils Warnken (University of Birmingham)*

MonPO-19 P00030 (19:30 ~ 21:00)

Rapid Estimation of the Liquidus Curve for Unexplored Multicomponent Alloy Chemistries

Joshua Willwerth, Shibo Tan, Abrar Rauf, and Wenhao Sun (University of Michigan)*

MonPO-20 P00032 (19:30 ~ 21:00)

An atomistic simulation study on ductility of amorphous aluminum oxide

Jisu Lee, Joonho Ji, Unyong Jeong, and Byeong-Joo Lee (POSTECH)*

MonPO-21 P00036

Thermodynamic Optimization of the Cr-C binary system using Modified Quasichemical Model

(19:30 ~ 21:00) *Muhammad Aiesh Ghayoor (Aalto University), Min-Kyu Paek* (Clausthal University of Technology), In-Ho Jung (Seoul National University)*

MonPO-22 P00037 (19:30 ~ 21:00)

Thermodynamic Modeling of Tramp Elements in Liquid Steel for The Sustainable Production of Steel

Won-Bum Park (POSTECH/Graduate Institute of Ferrous and Eco Materials Technology), Michael Christian Bernhard (Montanuniversität Leoben/Chair of Ferrous Metallurgy), Youn-Bae Kang (POSTECH/Graduate Institute of Ferrous and Eco Materials Technology)*

MonPO-23 P00038 (19:30 ~ 21:00)

Phase transformation of MnO_2 nanoparticles due to synthesis conditions, calcination temperature and duration

Reynald Ponte (Estonian University of Life Sciences), Durga Parajuli (National Institute of Advanced Industrial Science and Technology (AIST)), Larysa Khomenkova (National Academy of Sciences of Ukraine), Lisandra Da Rocha-Meneses (Estonian University of Life Sciences)*

MonPO-24 P00039 (19:30 ~ 21:00)

Experimental approaches for in situ determination of phase equilibria and thermodynamic properties above 2000 °C

Sergey V Ushakov, Jared Matteucci, and Alexandra Navrotsky (Arizona State University), Elizabeth J. Opila (University of Virginia)*

MonPO-25 P00040 (19:30 ~ 21:00)

Diffusion analysis in binary and ternary Ni-based alloys following Experimental, Density Functional Theory (DFT) and Physics-informed neural network numerical inverse method (PINN)

Ankur Srivastava (Indian Institution of Science), Suman Sadhu (Indian Institute of Science), Satyam Kumar and Ujjval Bansal (Indian Institution of Science), Ravi Raju (Indian Institute of Science), Saswata Bhattacharya (Indian Institute of Technology Hyderabad), Sai Gautam Gopalakrishnan and Aloke Paul (Indian Institution of Science)*

MonPO-26 P00043 (19:30 ~ 21:00)

The Cu-Ti system. The calorimetric studies of liquid alloys

Weronika Gozdur (Institute of Metallurgy and Materials Science Polish Academy of Sciences), Wojciech Gierlotka (National Dong Hwa University), Władysław Gąsior (Institute of Metallurgy and Materials Science Polish Academy of Sciences), Magda Pęska (Military University of Technology,), Adam Dębski (Institute of Metallurgy and Materials Science Polish Academy of Sciences)*

MonPO-

Integrated computational material engineering practice paths, from

27 P00044
(19:30 ~ 21:00)

CALPHAD to Phase Field and Crystal Plastic Finite Element

Xiaoyu Zheng (The School of Metallurgy and Environment, Central South University, China), Yong Du (The Powder Metallurgy Research Institute, Central South University, China)*

MonPO-28 P00048
(19:30 ~ 21:00)

Experimental study and thermodynamic modeling of B-Nb-Ta ternary system

Viera Homolova, Lucia Čiripová, and Frantisek Kromka (Institute of Materials Research, Slovak Academy of Sciences), Adéla Zemanová (Institute of Physics of Materials, Czech Academy of Sciences)*

MonPO-29 P00049
(19:30 ~ 21:00)

Improving cleanliness of low-carbon steel through modeling of BOF tapping operations

Rafaela P.B. Carvalho (CSN), Juila Mendes Sales (EEIMVR-UFF), Andre Luiz Costa e Silva (EEIMVR-UFF and IBQN), Rafaela P.M. Santos and Erica P. Silva (CSN), José Adilson Castro (EEIMVR-UFF)*

MonPO-30 P00073
(19:30 ~ 21:00)

Evaluating Steel Reoxidation by Atmospheric Oxygen Pickup in Deep Desulfurization in Ladle Furnace

Paulo Vinicius Toledo (EEIMVR-UFF), Gilberson Stork Melo and Miguel Liska Bock (GERDAU AÇOMINAS OURO BRANCO), Jose Adilson Castro (EEIMVR-UFF), Andre Luiz Costa e Silva (EEIMVR-UFF and IBQN)*

MonPO-31 P00055
(19:30 ~ 21:00)

Suppression of Detrimental Fe-Related Phases in Secondary Aluminum Alloys with CALPHAD-Guided Strategies

Chuan Zhang (CompuTherm LLC), Alan A Luo (The Ohio State University), Shuanglin Chen and Fan Zhang (CompuTherm LLC)*

MonPO-32 P00057
(19:30 ~ 21:00)

Computational study of zirconium oxidation using phase-field modeling

Jiho Kim and Kunok Chang (Kyung Hee University)*

MonPO-33 P00059
(19:30 ~ 21:00)

Thermodynamic calculation of alkali metal hydride systems for hydrogen storage

Jae-Hyeok Shim (Korea Institute of Science and Technology), Byeong-Joo Lee (Pohang University of Science and Technology), Young Whan Cho (Korea Institute of Science and Technology)*

MonPO-34 P00064 (19:30 ~ 21:00)

Solidification paths and phase equilibria in the X-Er-Y system (X=Al, Zr)

Ri Liu (Central South University), Xiaoxu Liu (CNPC Tubular Goods Research Institute), Yong Du (Central South University)*

MonPO-35 P00075 (19:30 ~ 21:00)

Understanding the electrochemical properties of Mg-doped Li_2MnO_3 from first-principles calculations

Jianchuan Wang (Central South University)*

MonPO-36 P00076 (19:30 ~ 21:00)

Experimental determination and thermodynamic assessment of the Co–Cr binary system

Kazushige Ioroi, Haruhi Kumeta, Xiao Xu, Ryosuke Kainuma, and Toshihiro Omori (Tohoku University)*

MonPO-37 P00077 (19:30 ~ 21:00)

Development of Phase Field Software MID-MESO with Application on U-Nb Discontinuous Precipitation Simulation

Zihang Wang (Central South University), Hong Mao (Hunan Institute of Science and Technology), Qi Huang and Yong Du (Central South University)*

MonPO-38 P00078 (19:30 ~ 21:00)

Phase formation in Ta-Mo-Cr-Ti-Al refractory high entropy alloys: CALPHAD-aided prediction and experimental study

Kateryna Khanchych and Bronislava Gorr (KIT)*

MonPO-39 P00081 (19:30 ~ 21:00)

Experimental and Theoretical Study of Phase Equilibria in the La-Ni-Sn system

Ales Kroupa (Institute of Physics of Materials, CAS, v.v.i., CZ68081723 Brno), Ondrej Zobac (Institute of Physics of Materials, CAS, Brno), Rudolf Zizka (Masaryk University, Brno), Martin Friak (Institute of Physics of Materials, CAS, Brno), Klaus W. Richter (Universitat Wien), Bedrich Smetana (VSB Technical University, Ostrava,)*

MonPO-40 P00083 (19:30 ~ 21:00)

Experimental investigation and thermodynamic assessment of Cr-Mo-Si ternary system

Arun Ramasamy Chitra and Bronislava Gorr (Karlsruhe Institute of Technology)*

MonPO-41 P00087 (19:30 ~ 21:00)

Phase-Field Modeling of How Porosity and Sodium Infiltration Influence Constituent Redistribution in U-Zr Metallic Fuels

Woojin Jung (Kyung Hee University), Juseong Kim (Korea Atomic Energy Research Institute), Kunok Chang (Kyung Hee University)*

MonPO-42 P00090 (19:30 ~ 21:00)

Phase-field Simulation of Phase Transformation of Carbidesin Ni-Mo-C system

Woojien Lee and Kunok Chang (Kyung Hee University)*

MonPO-43 P00091 (19:30 ~ 21:00)

Predicting the terminal solid solubility of hydrogen in Zr-alloy cladding using machine learning approach and phase-field modeling

Sanghyun Ji and Kunok Chang (Kyung Hee University)*

MonPO-44 P00092 (19:30 ~ 21:00)

Experimental investigation on phase equilibrium and thermodynamic property of the CaO-Fe_2O_3-TiO_2 system in air

Mengjiao Jiao and Yang Zhang (Chongqing University), Guishang Pei (Seoul National University), Zhuoyang Li and Xuewei Lv (Chongqing University)*

MonPO-45 P00093 (19:30 ~ 21:00)

Experimental measurement of equilibrium between molten copper and magnesium-phosphate

Shunsuke Watanabe, Hiroshi Fukaya, and Takahiro Miki (Tohoku university)*

MonPO-46 P00094 (19:30 ~ 21:00)

Effect of Tramp Elements on Cu-rich Liquid Phase Formation in the Hot-Rolling Process

Minseo Cho, EunEui Lee, Ikhyeon Cho, Yeonjee Choi, and Joonho LEE (Korea University)*

MonPO-47 P00095 (19:30 ~ 21:00)

Computational Design of Mg Alloys with Minimal Galvanic Corrosion

Krishnamohan Thekkepat (Korea Institute of Science and Technology), Pil-Ryung Cha (Kookmin University), Seung-Cheol Lee (Korea Institute of Science and Technology)*

MonPO-

In-situ HEXRD study on the β-α transformation in Al 6063

48 P00096
(19:30 ~ 21:00)

Nicolás García Arango and Erwin Povoden-Karadeniz (TU Wien)*

MonPO-49 P00097
(19:30 ~ 21:00)

Development and Application of a Deep Neural Network Potential for Cu-Sn Alloys

Jae Hur (Inha university), Won-Seok Ko (Inha University)*

MonPO-50 P00099
(19:30 ~ 21:00)

Thermodynamic re-assessment of LiCl-$GdCl_3$ molten salt system

K L Anantha Krishna (University of Hyderabad), Sajal Ghosh (Indira Gandhi Centre for Atomic Research), Soumya Sridar (Indian Institute of Technology Kanpur), Rajesh Ganesan (Indira Gandhi Centre for Atomic Research; Homi Bhabha National Institute), K Guruvidyathri (University of Hyderabad)*

MonPO-51 P00107
(19:30 ~ 21:00)

Experimental, DFT, stability and site occupancies investigation of selected TCP A15 phases

Chancel Mawalala Moundounga, Ahmed Aissaoui, and Celine Barreteau (CNRS), Mariano Forti and Thomas Hammerschmidt (ICAMS), Jean-Claude Crivello (LINK), Jean-Marc Joubert (CNRS)*

MonPO-52 P00111
(19:30 ~ 21:00)

Developing High Strength, High Toughness Naval Steels:10Ni-150

You Na Lee, Cole Jared Kuehmann, Cemal Cem Tasan, and Gregory B. Olson (Massachusetts Institute of Technology)*

MonPO-53 P00114
(19:30 ~ 21:00)

Graph Neural Network (GNN)-Based Framework Integrating Positive and Unlabeled (PU) Learning for Accurate Prediction of Hardness and Modulus in High-Entropy Alloys

Aamir Malik and Ho Jin Ryu (Korea Advanced Institute of Science and Technology (KAIST))*

TuePO - Poster session (2)

May 27 (Tue), 19:30-21:00, Sydney Room

Session Chair:

TuePO-1 P00118
(19:30 ~ 21:00)

Optimization of Slag Chemistry in EAF operations for Enhanced Sustainability

Nuga YOON, Juyeong LEE, and Joonho LEE (Korea University)*

TuePO-2 P00119 (19:30 ~ 21:00)
Which Calphad Database Should We Use? — Strategic Selection for Materials Design in Additive Manufacturing

Marcia Myung Hye Ahn, Soumya Sridar, Luis Fernando Ladinos Pizano, and Wei Xiong (University of Pittsburgh)*

TuePO-3 P00121 (19:30 ~ 21:00)
Development of a Web Platform for Large-Scale Thermodynamic Calculations and Data Accessibility

Min-Ho Lee, Min-Kyu Park, Jung-Ho Lee, and Young-Kwang Kim (Virtuallab Inc.)*

TuePO-4 P00122 (19:30 ~ 21:00)
Phase Transition of Gangue Materials during Reduction of Iron Ore by Hydrogen-enriched Gas

DAVIN MYEONG, Eunju Kim, In kook Suh, and Joonho LEE (Korea University)*

TuePO-5 P00124 (19:30 ~ 21:00)
Design of High-Entropy Alloy Interlayers to Control Intermetallic Compounds in Multi-Materials Joining

Yoona Lee, Seonghoon Yoo, Byoungwook Choi, Wookjin Lee, Yoon suk Choi, and Namhyun Kang (Pusan National University)*

TuePO-6 P00125 (19:30 ~ 21:00)
Phase-field Model to Simulate Microstructural Evolution Behavior of Fe-Cr-Ni Alloy

Jeonghwan Lee and Kunok Chang (Kyung Hee University)*

TuePO-7 P00127 (19:30 ~ 21:00)
Correlation between N_2O Sensing Performance and DFT Adsorption Energy in Metal Oxide Semiconductors

JeongMin Lee, Sangwoo Kim, and DongEung Kim (Korea Institute of Industrial Technology), Kee-Sun Sohn (Sejong University)*

TuePO-8 P00128 (19:30 ~ 21:00)
Experimental study and thermodynamics of the Na^+, K^+, Mg^{2+}, Ca^{2+} // Cl^-, SO_4^{2-} multi-component system

Amedeo Morsa and Elena Yazhenskikh (Forschungszentrum Jülich), Dmitry Sergeev (NETZSCH-Gerätebau GmbH), Rhys Jacob and Michael Müller (Forschungszentrum Jülich)*

TuePO-9 P00132 (19:30 ~ 21:00) **Evaluation of liquid metal embrittlement resistance of Zn-coated steels via thermodynamic approach**

Daehoon Jeong (POSTECH), Sang-Ho Oh (Pohang University of Science and Technology), Byeong-Joo Lee and Sung-Joon Kim (POSTECH (Pohang University of Science and Technology))*

TuePO-10 P00133 (19:30 ~ 21:00) **Comparison of Cracking Characteristics of Al-Zn-Mg-Cu Alloy in DED and PBF Processes Using a Novel Cracking Susceptibility Model**

Matae Lee (POSTECH (Pohang University of Science and Technology)), Soobin Kim (Inha University), Man Jae SaGong (POSTECH (Pohang University of Science and Technology)), Kee-Ahn Lee (Inha University), Hyoung Seop Kim and Byeong-Joo Lee (POSTECH (Pohang University of Science and Technology))*

TuePO-11 P00135 (19:30 ~ 21:00) **CALPHAD-Informed Gaussian Process Classification for Constraint-Aware Alloy Design**

Brent Garrett Vela, Christofer Hardcastle, and Raymundo Arroyave (Texas A&M Materials Science)*

TuePO-12 P00136 (19:30 ~ 21:00) **Thermodynamic properties of the Sb_6O_{13} and $Ca_6Sb_2O_{11-\sigma}$**

Shu Li, Wenjie Wei, and Zhanmin Cao (University of Science and Technology Beijing)*

TuePO-13 P00137 (19:30 ~ 21:00) **Evaluation of Plastic Waste as a Carbon Additive in Slag Foaming Reactions for Sustainable Steelmaking**

HYOJU AHN and Nokeun Park (Yeungnam University), Youngjo Kang and Sangcheol Sim (Dong-A University), Eunjin Lee and Hyomin Kim (Materials Solution Park)*

TuePO-14 P00138 (19:30 ~ 21:00) **Thermodynamic Prediction of Elemental Loss During Additive Manufacturing: A Calphad Approach with Supporting Experiments**

Marcia Myung Hye Ahn, Soumya Sridar, and Wei Xiong (University of Pittsburgh)*

TuePO-15 P00142 (19:30 ~ 21:00) **Thermodynamic behavior of TiO_2 in CaO-Al_2O_3-MgO-TiO_2 slag at 1823 K**

Dongyul Jung, Yeongjin Jun, and Minjoo Lee (Hanyang University),

Sungjin Park and Suchang Kang (POSCO Technical Research Laboratories), Younbae Kang (POSTECH), Joohyun Park (Hanyang University)*

TuePO-16 P00145 (19:30 ~ 21:00) **Generalisation of model of interaction between intrinsic hydrogen and moving heat sources.**

Jack Richard Leeman and Nils Warnken (University of Birmingham)*

TuePO-17 P00146 (19:30 ~ 21:00) **Model form and sensitivity analysis of CALPHAD-based nucleation models in beta-stabilized Ti alloys**

Aaron Tallman, Astrid Michelle Rodriguez Negron, and Audrey Torres (Florida International University)*

TuePO-18 P00147 (19:30 ~ 21:00) **Enhancing Accuracy in Configurational Entropy Calculations with Correlation Correction for Complex Systems**

Dallin Jackson Fisher and Qijun Hong (Arizona State University)*

TuePO-19 P00148 (19:30 ~ 21:00) **New findings in the K_2O-SiO_2-CO_2 system: phase relations and experimental observations**

Maria Ilatovskaya, Elena Yazhenskikh, Mirko Ziegner, Inge Dreger, and Michael Mueller (Forschungszentrum Juelich)*

TuePO-20 P00150 (19:30 ~ 21:00) **Experimental study on interaction of KCl with potassium silicates and re-assessment of the K_2O-SiO_2 system**

Elena Yazhenskikh, Maria Ilatovskaya, Mirko Ziegner, and Michael Mueller (Forschungszentrum Juelich)*

TuePO-21 P00161 (19:30 ~ 21:00) **Thermodynamic insights on MgO solubility in Li_2O-containing iron-silicate melts**

Sehyeon Nam and Joohyun Park (Hanyang University)*

TuePO-22 P00163 (19:30 ~ 21:00) **Experimental Investigation and Thermodynamic Optimization of the Co–Fe–Nb System**

Zhenmin Du (University of Science and Technology Beijing)*

TuePO-23 P00167 (19:30 ~ 21:00) **Design of Oxidation Resistant Alloys using Combinatorial Approaches with Chemically Graded Materials**

Sabrina Ghanes and Mikael Perrut (ONERA), Enrica Epifano (CIRIMAT), Matthieu Degeiter (ONERA), Thomas Vaubois (SAFRAN-Tech), Yohan Cosquer (DGA), Daniel Monceau (CIRIMAT)*

TuePO-24 P00168 (19:30 ~ 21:00) **Exploration of high-ductility quinary refractory high-entropy alloys**

Hyo-Sun Jang (Korea Institute Of Materials Science), Jin-Woong Lee (SK Siltron Inc.), Sujung Son (Pohang University of Science and Technology), Byung Do Lee (Sejong University), Jiwon Park (Korea Institute of Materials Science), Kee-Sun Sohn (Sejong University), Hyoung Seop Kim (Pohang University of Science and Technology), Chang-Seok Oh (Korea Institute of Materials Science)*

TuePO-25 P00169 (19:30 ~ 21:00) **Estimation of specific heat capacity and thermal conductivity of Fe-SiO_2 mixture using laser flash analysis**

Yuncheol HA and Joonho LEE (Korea University)*

TuePO-26 P00172 (19:30 ~ 21:00) **Molecular dynamics simulation study on the additively manufactured shape-memory alloys**

Jong-Hoon Park and Won-Seok Ko (Inha University)*

TuePO-27 P00173 (19:30 ~ 21:00) **Phase Transformation and Structural Ordering in Mg-Sc Shape Memory Alloys: A First-Principles Approach**

Hye-Hyun Ahn (Inha university), Won-Seok Ko (Inha University)*

TuePO-28 P00174 (19:30 ~ 21:00) **Thermodynamics of titanium distribution between ferrosilicon melt and CaO-SiO_2-Al_2O_3 slag at 1773 K**

Minjoo Lee and Joohyun Park (Hanyang University)*

TuePO-29 P00177 (19:30 ~ 21:00) **Deep Potential for $TiMn_2$-based hydrogen storage alloys**

HUNMIN JO (INHA University), Won-Seok Ko (Inha University)*

TuePO-30 P00178 (19:30 ~ 21:00) **Prediction of Elastic Properties of Refractory HEAs by Machine Learning with Uncertainty Quantification**

Chang-Seok Oh, Hyo-Sun Jang, and Jiwon Park (Korea Institute of*

Materials Science)

TuePO-31 P00179 (19:30 ~ 21:00) **First-principles investigation of solute atom effects on the hydrogen storage properties of Mg_2Ni**

Min-Seok Yoon (Inha Unviersity), Won-Seok Ko (Inha University)*

TuePO-32 P00180 (19:30 ~ 21:00) **Thermo-kinetic insights into low-temperature recycling of lithium iron phosphate (LFP) batteries via graphite reduction**

Yuri Kim and Il Sohn (Yonsei University)*

TuePO-33 P00182 (19:30 ~ 21:00) **Experimentally based optimization of interaction parameters in G-phase in Fe-Si-Ni-Mn system**

Evgenii Meshkov (FSUE VNIIA), Irina Bajenova and Vladimir Cheverikin (Lomonosov MSU, Faculty of Chemistry), Alexey Yanilkin (FSUE VNIIA), Alexandra Khvan (Lomonosov MSU, Faculty of Chemistry)*

TuePO-34 P00183 (19:30 ~ 21:00) **Integrated DFT and machine learning study on hydrogen storage properties of C14 type high-entropy alloys**

Seo-Hui Park (Inha university), Won-Seok Ko (Inha University)*

TuePO-35 P00184 (19:30 ~ 21:00) **High Temperature Deformation Mechanism of LWDED Processed IN625 According to Flow Stress Direction**

Minho Kim and SOHN Il (Yonsei University)*

TuePO-36 P00185 (19:30 ~ 21:00) **Equilibrium solubility of hydrogen in molten alloys**

Junyoung Kim, Ji won Im, Hui Duk Yoo, Chang Hun Keum, Sang Chul Shim, and youngjo Kang (Dong-A University)*

TuePO-37 P00187 (19:30 ~ 21:00) **Integrated Microstructure-Property Prediction in Structural Alloys Through Multi-Modal Machine Learning**

Jiwon Park and Chang-Seok Oh (Korea Institute of Materials Science), Joo-Hee Kang (WAVESENSE), Su-Hyeon Kim (Korea Institute of Materials Science)*

TuePO-38 P00194 (19:30 ~ 21:00) **Thermodynamic Prediction of Iodides for Molten Salt Reactor Operation**

Yongjin Cho and In-Ho Jung (Seoul National University)*

TuePO-39 P00195 (19:30 ~ 21:00) **Rocket Performance Estimation with Regolith-Derived Propellants using FactSage**

Harim Kim and Marie-Aline van Ende (Seoul National University), Xiaocheng Mi (Eindhoven University of Technology), In Ho Jung (Seoul National University)*

TuePO-40 P00198 (19:30 ~ 21:00) **Critical Evaluation and Optimization of the BaO-TiO_2-Ti_2O_3 System**

Taehyoung Kim and In-Ho Jung (Seoul National University)*

TuePO-41 P00199 (19:30 ~ 21:00) **Evaluation of Microstructure and Thermodynamic Analysis of Rapidly Solidified Cu-Sn Alloys**

Wu Dinghao, Tang Yongpeng, Akamine Hiroshi, Shimada Yusuke, and Ishibashi Ryo (Kyushu University), Tokunaga Tatsuya (Kyushu Institute of Technology), Iikubo Satoshi (Kyushu University)*

TuePO-42 P00202 (19:30 ~ 21:00) **Coupled Experiments and Thermodynamic Modelling for the MgO-SiO_2-Nb_2O_5 System**

Akshat Pachauri and In-Ho Jung (Seoul National University)*

TuePO-43 P00204 (19:30 ~ 21:00) **Thermodynamic Analysis of the Ba-Ca-Mg-F Quaternary system**

YuXuan Ho and Yongpeng Tang (Kyushu University), Kousuke Noi (Kyoto University), Hidenori Miki (Toyota Motor Corporation), Satoshi Iikubo (Kyushu University)*

TuePO-44 P00206 (19:30 ~ 21:00) **Deep understanding of phase equilibria and CALPHAD modelling in Ti-Al-X (X=Nb, Mo, W, Si, Zr, O, B, C) systems**

Yang Yang, Anders Engstrom, Hai-Lin Chen, and Qing Chen (Thermo-Calc Software)*

TuePO-45 P00207 (19:30 ~ 21:00) **Effect of Dew Point during Annealing on Phosphatability of Ultra-High-Strength Steel**

Joongchul Park (POSCO), Jiwoo Park (Korea University), Yoon-Uk Heo

(Pohang University of Science and Technology), Yeongyun Song (POSCO), Joonho Lee (Korea University)*

TuePO-46 P00208 (19:30 ~ 21:00) **Experimental Determination of Liquidus Temperature of the CaO-Fe_2O_3 Binary System under Different Oxygen Partial Pressures**

Haeun Kim and Joonho Lee (Korea University)*

TuePO-47 P00209 (19:30 ~ 21:00) **Improving joint strength of lightweight magnesium and aluminum joints by depositing a third element**

Mingzhe Bian and Ryoichi Furushima (National Institute of Advanced Industrial Science and Technology)*

TuePO-48 P00210 (19:30 ~ 21:00) **Thermodynamics of Ni distribution between liquid copper and CaO-SiO_2-Fe_tO-MgO slag**

Sumin Hwang and Joo Hyun Park (Hanyang University)*

TuePO-49 P00213 (19:30 ~ 21:00) **Thermodynamic Modeling of Pure Elements from 0 K with Uncertainty Quantification using PyCalphad and ESPEI**

Alexander Richter (Penn State University), Irina Roslyakova (Ruhr-Universitat Bochum), Allison Beese and Zi-Kui Liu (Penn State University)*

TuePO-50 P00218 (19:30 ~ 21:00) **A new interface for Effective Equilibrium Reaction Zone (EERZ) in FactFlow**

Kyota Poeti (Polytechnique Montréal), André Costa e Silva (Escola de Engenharia Industrial Metalúrgica de Volta Redonda - Universidade Federal Fluminense), Kentaro Oishi and Jean-Philippe Harvey (Polytechnique Montréal)*

TuePO-51 P00220 (19:30 ~ 21:00) **Effective Bond Energy Formalism Description of the μ Phase in the Co-Cr-Ni-W System**

Julio Cesar Pereira dos Santos (Thermo-Calc Software), Ursula R Kattner (National Institute of Standards and Technology)*

TuePO-52 P00222 (19:30 ~ 21:00) **Mechanism of Microwave-Induced Pyrite Removal from Coal: A Synergistic Study Combining Thermodynamic Calculations and Density Functional Theory**

Yucen Kuang, Shengfu Zhang, Chenguang Bai, Buxin Chen, and Meilong Hu (Chongqing University)*

TuePO-53 P00224 (19:30 ~ 21:00) **Theory and Application of Predictive Molecular Thermodynamics**

Guoxuan Li, Pan Xu, and Yinglong Wang (Qingdao University of Science and Technology)*

TuePO-54 P00225 (19:30 ~ 21:00) **Calphad extended to electrochemical diagrams showing equilibrium cathodic phases and their compositions as function of electrolyte composition at low current densities**

George Kaptay (Uni Miskolc)*

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Accommodation and meals

1. Notice of reservation

- For **general participants and students with hotel**, the registration fee includes
  - All sessions, book of abstracts
  - Breakfast, lunch, dinner and coffee breaks at Paradise Hotel from Monday morning to Friday lunch
  - Welcome reception on Sunday
  - Excursion
  - Conference Banquet
  - Hotel includes the 5 nights from May 25 (check-in) to 30 (check-out)
  - Single free ticket for Simer (Ocean Spa)

- For **accompanying person** (general participant must stay in the Paradise Hotel), the registration fee includes
  - Breakfast, lunch, dinner and coffee breaks at Paradise Hotel from Monday morning to Friday lunch
  - Welcome reception on Sunday
  - Excursion
  - Accompanying persons tours (For some options, additional cost can be applied)
  - Conference Banquet
  - Single free ticket for Simer (Ocean Spa)

- For **general participants and students without hotel**, the registration fee includes
  - All sessions, book of abstracts
  - Lunch, dinner and coffee breaks at Paradise Hotel from Monday morning to Friday lunch
  - Welcome reception on Sunday
  - Excursion
  - Conference Banquet

2. Accommodation

- Paradise Hotel Busan | 296, Haeundaehaebyeon-ro (Jung-dong), Haeundae-gu, Busan, Korea, +82-51-742-2121 | E-mail: welcome@paradian.com
- https://www.busanparadisehotel.co.kr/front
- Simer: https://www.busanparadisehotel.co.kr/front/facility/spaparacimer
- Kids activities in hotel: https://www.busanparadisehotel.co.kr/front/facility/kidsList

- For registered participants with hotel, check-in can be done individually and will be available from 3 PM.

2. Meals

- **Breakfast (only for general participants and students with hotel)**
  - Business hours: 6:30 ~ 10:00 AM
  - Place: On the plate, Main Building 1F, Paradise Hotel Busan (https://www.busanparadisehotel.co.kr/front/facility/dinebuffet)
  - You can enter by stating your room number and name.

- **Lunch and Dinner (all participants, from May 26 to May 30, except dinners on May 28 and May 29)**
  - Place: Capri room, Main Building 2F, Paradise Hotel Busan

- **Welcome reception (all participants, May 25)**
  - Place: Sicily room & Garden, Main Building 2F, Paradise Hotel Busan
  - Only Snacks & Beverages will be provided

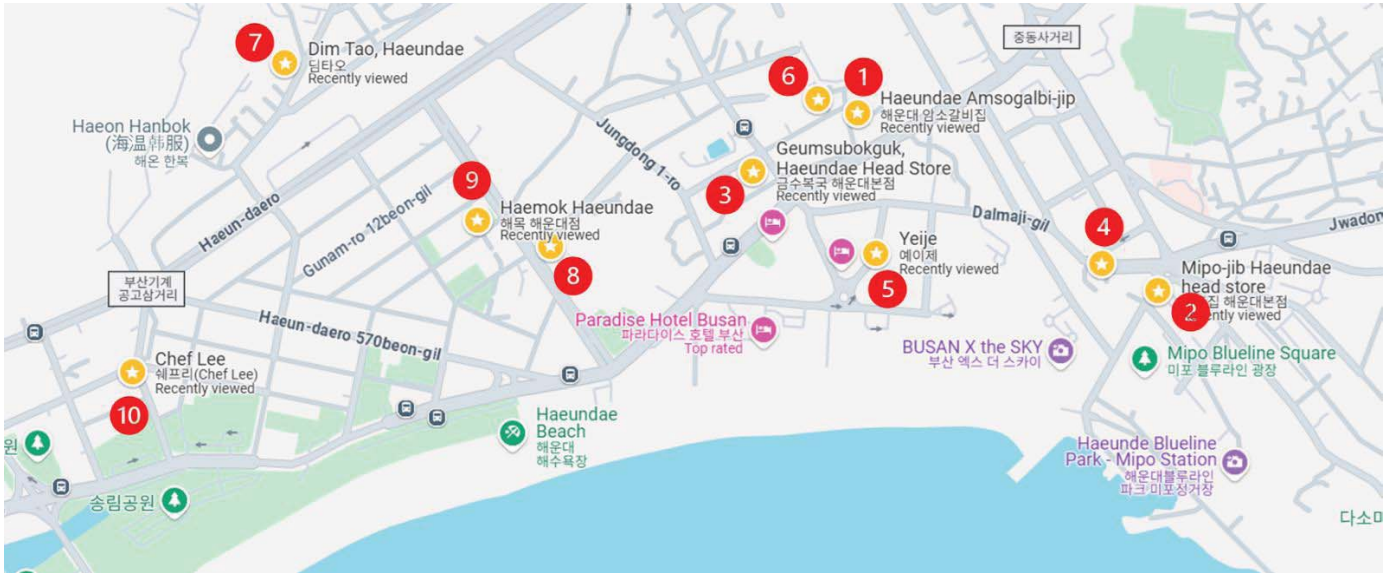
- **Banquet (all participants, May 29)**
  - Place: Grand ballroom, Main Building 2F, Paradise Hotel Busan

* Participants who have submitted **dietary requests** in advance are kindly asked to **collect their dietary name cards from the staff at the entrance of the Capri Room or the Grand Ballroom before entering.**

Please **place your dietary name card on the table** so that we can provide meals according to your requested dietary preferences. (In normal case, no plate is required).

Secretariat will inform each participant who submitted their specific meal type via individual email.

Recommended Restaurants



1. **Haeundae Amsogalbi-jip (해운대 암소갈비집)**:
   https://maps.app.goo.gl/Er5NG7WtS2BAGiRz8
   Michelin Guide Busan, Korean-style BBQ specializing in beef short ribs

2. **Mipo-jib Haeundae head store (미포집 해운대본점)**:
   https://maps.app.goo.gl/iUWEYGZMX9rkVYQ87
   Korean-style steamed seafood, combining fresh seafood with flavorful seafood sauces

3. **Geumsubokguk, Haeundae Head Store (금수복국 해운대점):**
   https://maps.app.goo.gl/rP4eCYPr4nGywDo2A
   A restaurant specializing in puffer fish cuisine, and featured in the Michelin Guide

4. **Busan Tteun Mackerel Haeundae Branch (부산에뜬고등어 해운대점)**:
   https://maps.app.goo.gl/25mQHmDnodYWLidv5
   Korean-style grilled fish and traditional Korean set meals

5. **Yeyje (예이제)**: https://maps.app.goo.gl/7tDDLUrPJPgXv3tu8
   Korean traditional fine dining featuring premium ingredients.

6. **Haeundae Wheat Noodles (해운대밀면)**:
   https://maps.app.goo.gl/dTGCSJSNguSXNtsC6
   Traditional Korean cold noodle restaurant

7. **Dim Tao, Haeundae (딤타오 해운대)**:
   https://maps.app.goo.gl/1yFNNm7hkM8wEicP7
   Michelin Guide-listed restaurant known for authentic Chinese dim sum

8. **Hi asia Indonesian restaurant (하이아시아)**:
   https://maps.app.goo.gl/6skhaoTcTeC8yQSc6
   Indian cuisine specializing in tasty naan bread and flavorful curries

9. **Haemok Haeundae (해목 해운대)**: https://maps.app.goo.gl/kuQ8BopnS4NJnupe9
   Michelin Guide-listed Japanese restaurant specializing in rice bowls (donburi) and eel rice bowls (unadon)

10. **Chef Lee (쉐프리)**: https://maps.app.goo.gl/nGs1bih6gr1qYFdW7
    Italian restaurant serving delicious pizza, pasta, and more.