CALPHAD L Conference Program Summary for Oral Presentations, Version 1.4, Updated on 5/17/2023

This program may be updated further if any presenter has to cancel the talk due to visa issues

Please make sure to check the latest version online: https://calphad.org/calphad-2023

No.	start	duration, min	Session Chair	First name	Last name	Abstract Title
	8:00	0:10		Yu Zhong & Wei Xiong		Openning
Monday	**6/25/2023**	**Session 1**	**CALPHAD: Past, Current, and Future**			
1	8:10	0:20		Gregory	Olson	Materials Genomics: Honoring the Vision of Larry Kaufman
2	8:30	0:20		John	Ågren	Mats Hillert and CALPHAD – a memorial tribute
3	8:50	0:20	Yu Zhong, Wei Xiong	Zi-Kui	Liu	Towards the integration of quantum, statistical, and irreversible thermodynamics for accurate prediction of free energy landscape and kinetic properties
4	9:10	0:20		Bo	Sundman	Developing Models and Software for 50 years
5	9:30	0:20		Malin	Selleby	3rd generation models – review and way forward
6	9:50	0:25		Charles	Kuehmann	CALPHAD for a Better Planet and an Interplanetary Future
Break	**10:15**	**0:30**	**CALPHAD Modeling and Database Development (I)**			
7	10:45	0:20		Bengt	Hallstedt	Thermodynamic database for multi-principal element alloys within the system Al–Co–Cr–Fe–Mn–Ni–C(–V)
8	11:05	0:20		Julian	Gebauer	Thermodynamic assessment of ternary Al-M-O (M= Nb, Ta) systems
9	11:25	0:20	Rainer Schmid-Fetzer, Malin Selleby	Aurélie	Jacob	Thermodynamic prediction of the C-dependency for bainite formation: the importance of Fe-C
10	11:45	0:20		Lucas	Tosin Paese	Assessment on the Li-Ni-Mn-Co-O System and Applications on Lithium-Ion Batteries Layered Cathodes
11	12:05	0:20		Zhi	Liang	Development of QuesTek Databases for Integrated Computational Material Design
Monday	**6/25/2023**	**Session 2**	**Atomistic Modeling and Prediction (I)**			
12	14:00	0:20		Mira	Todorova	Using ab-initio phase diagrams to tune experimental synthesis routes
13	14:20	0:20		Hiroshi	Ohtani	Construction of the Theoretical Phase Diagrams Based on the First-Principles Calculation
14	14:40	0:20	Andre Costa e Silva, Jooho Lee	Shigeto	Nishitani	Finite temperature boundary energy of Al
15	15:00	0:20		Songge	Yang	Ab Initio Modeling on The Thermodynamic and Temperature-Dependent Elastic Properties of Subsystems of The FCC FeNiCoCr Medium Entropy Alloys (MEAs)
16	15:20	0:20		Yu-ning	Chiu	High Temperature Al-Zn-Mg Alloys Design: High-throughput DFT Calculations and Machine Learning
Break	**15:40**	**0:30**	**CALPHAD Applications (I)**			
17	16:10	0:20		Hans Jürgen	Seifert	Lithium-ion Batteries Studied by Calorimetry and CALPHAD
18	16:30	0:20		Andre	Costa e Silva	Insights into improving steel secondary metallurgy using computational thermodynamics
19	16:50	0:20		Ping	Wu	Approaching Multiphysics Problems from Entropy
20	17:10	0:20	Bengt Hallstedt, Dongwon Shin	Lorenzo	Fenocchio	Validation and Application of the Genova High-Entropy Alloys (GHEA) Thermodynamic Database for Selected Multi-component Systems
21	17:30	0:20		Hui	Sun	Feasibility Map: A CALPHAD-Based Approach to Design Composition Pathway for Desired Dissimilar Materials Processed by Casting, Welding and Additive Manufacturing

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Tuesday	**6/26/2023**	**Session 3**	**CHiMaD Sponsored session: Materials Genome and Materials Design (I)**			
22	8:00	0:25		James	Warren	The Materials Genome Initiative: Reaching for Impact
23	8:25	0:20		Ursula	Kattner	CALPHAD models: quo vadis?
24	8:45	0:20		Noah	Paulson	CALPHAD Uncertainty Quantification: Problems and Solutions
25	9:05	0:20	John Ågren, Sinn-wen Chen	Changning	Niu	CALPHAD Uncertainty Quantification and Design with Uncertainty
26	9:25	0:20		Adetoye	Adekoya	Shapes of Single-Phase Diagrams
27	9:45	0:20		Christopher	Hareland	A CALPHAD model of non-equilibrium plane-front and dendritic growth in concentrated multicomponent alloys
Break	**10:05**	**0:30**	**CHiMaD Sponsored session: Materials Genome and Materials Design (II)**			
28	10:35	0:20		Pereira dos Santos	Julio Cesar	Development of a thermodynamic database for Co-based superalloys.
29	10:55	0:20	Qing Chen, Shih-kang Lin	Krista	Biggs	Printable Co Superalloys Exploiting Multiphase Precipitation Strengthening for Strain-Age Cracking Resistance
30	11:15	0:20		Florian	Hengsbach	Printable Die Steel for GigaCasting
31	11:35	0:20		Julian	Rackwitz	High-strength high-damping steels: A CALPHAD assisted alloy design study
32	11:55	0:25		David	Furrer	ICME applications in Pratt & Whitney
Tuesday	**6/26/2023**	**Session 4**	**CALPHAD Applications (II)**			
33	14:00	0:20		Joonho	Lee	Development of Grade 700 MPa High-Strength Seismic Rebars by Integrated Computational Materials Engineering and Machine Learning
34	14:25	0:20	Scott McCormack, Bi-Cheng Zhou	S. Mohadeseh	Taheri-Mousavi	Physics-constrained, inverse design of high-temperature, high-strength, creep-resistant printable Al alloys using machine learning methods
35	14:45	0:20		Dimitra	Spathara	Modelling elemental surface sublimation of single crystal Ni-based superalloys at high temperatures
36	15:05	0:20		Mario J.	Kriegel	CalPhaD-Assisted Alloy Design for Fe-based Shape Memory Alloys
37	15:25	0:20		Joseph	Moses	Modelling reactions between ceramic oxides and Ti-Al melt
Break	**15:45**	**0:30**	**CALPHAD Applications (III)**			
38	16:15	0:20		Dongwon	Shin	High-throughput CALPHAD to Augment Scientific Features in Modern Data Analytics for Advanced Alloy Design

39	16:35	0:20		Adam	Krajewski	Alloy Data Quality Assurance Tools in ULtrahigh TEmperature Refractory Alloys (ULTERA) Database
40	16:55	0:20	Nils Warnken, Alexander Pisch	Michael	Bernhard	Development of a thermodynamic database for future control of tramp elements in steelmaking processes
41	17:15	0:20		Daozheng	Li	New feedstock design for additive manufacturing using a commercial alloy powder mixture
42	17:35	0:20		Guangchen	Liu	High-Entropy Materials Design by Integrating the First-Principles Calculations and Machine Learning: A Case Study in the Al-Co-Cr-Fe-Ni System
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Wednesday	**6/27/2023**	**Session 5**	**Experimental Equilibria and Phase Transformations**			
43	8:00	0:20		Alexandra	Navrotsky	How experimental thermochemistry can help actinide theory and phase equilibria.
44	8:20	0:20		Scott	McCormack	Enthalpy of mixing in entropy stabilised oxides
45	8:40	0:20	Andre Schneider, Stephanie Lippmann	Alexander	Pisch	Heat of dissolution & standard heat of formation of oxides using high temperature calorimetry
46	9:00	0:20		Sinn-wen	Chen	Eutectic and liquidus temperatures of Sn-based alloys
47	9:20	0:20		Sergey	Ushakov	Structure and thermodynamics of ceramics above 2000 °C
48	9:40	0:20		Jeong-Min	Cheon	Coupled Phase Diagram Experiment and Thermodynamic Modeling of the La2O3-MgO-SiO2 System
Break	**10:00**	**0:30**	**Atomistic Modeling and Prediction (II)**			
49	10:30	0:20		Jörg	Neugebauer	Metastable defect phase diagrams as road map for defect design
50	10:50	0:20		Ying	Chen	Stability of FeNiCoCrMnAlx and FeNiCoCrPdAlx:fully disordering vs. partially disordering
51	11:10	0:20	Raymundo Arróyave, Theresa Davey	Wei	Chen	Design metastability in high-entropy alloys by tailoring unstable fault energies
52	11:30	0:20		Yi	Wang	A Parameter-Free First-Principles-Based Debye Model to Predict Thermodynamic Properties of Complex Alloy Systems
53	11:50	0:20		Lifang	Zhu	Towards high throughput melting property calculations with ab initio accuracy aided by machine learning potential
Wednesday	14:00		Excursion & social events: Duck Tour Boarding 2:00 PM.			
	18:00		Dinner			
	19:00		Young Calphadian night starting from 7:00 PM			
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Thursday	**6/28/2023**	**Session 6**	**Diffusion and Phase Transformations**			
54	8:00	0:20		Qing	Chen	From PE to OE: Cementite Precipitation Pathway in Steels
55	8:20	0:20		Nils	Warnken	A Phase Field Model Based on Absolute Reaction Rate Theory
56	8:40	0:20		Takao	Suzuki	Thermodynamic investigation on the formation of G.P. zone in the Al-Cu binary system
57	9:00	0:20	Ping Wu, Karin Frisk	George	Kaptay	Beyond the parallel tangent method to predict composition of the first nucleating phase from oversaturated solutions
58	9:20	0:20		Clément	Introïni	PLEIADES/ALCYONE simulations of irradiated fuel thermochemistry coupled with oxygen thermal diffusion
59	9:40	0:20		Qi-Jun	Hong	Deep Learning for Large-Scale Prediction of Melting Temperature and Materials Properties
Break	**10:00**	**0:30**	**CALPHAD Modeling and Database Development (II)**			
60	10:30	0:20		Rainer	Schmid-Fetzer	3rd generation unary descriptions at high temperature
61	10:50	0:20		Raymundo	Arróyave	Uncertainty Quantification and Propagation in CALPHAD and CALPHAD-based Frameworks
62	11:10	0:20	Soumya Sridar, Dimitra Spathara	Jean-Marc	Joubert	Site occupancies in the quinary Co–Cr–Fe–Mn–Ni s phase
63	11:30	0:20		Shuanglin	Chen	Calculation of Spinodal and Critical Point in Multicomponent Systems
64	11:50	0:20		Arkapol	Saengdeejing	First-principles Thermodynamic Database for the Al-Ni-Ti
Thursday	**6/28/2023**	**Session 7**	**Thermodynamic Software and Model Development**			
65	14:00	0:20		Jean-Philippe	Harvey	A virtual laboratory for the aluminum industry
66	14:20	0:20		Andre	Schneider	The new Thermo-Calc Additive Manufacturing Module
67	14:40	0:20	Shuanglin Chen, Ursula Kattner	Bi-Cheng	Zhou	A Cluster-Based Computational Thermodynamics Framework with Intrinsic Chemical Short-Range Order
68	15:00	0:20		Florian	Tang	New strategies for thermodynamic equilibria in Calphad optimizations
69	15:20	0:20		Samuel	Krimmel	Novel Model for Gibbs Free Energy and Conductivity in Space Charge Layers Utilizing the CALPHAD Method
Break	**15:40**	**0:30**	**Thermodynamic Modeling, CALPHAD Database and Design Applications (I)**			
70	16:10	0:20		Gustavo	Costa	Thermochemical Modeling of Nuclear Thermal Propulsion Fuel Materials
71	16:30	0:20	Richard Otis, Zhi Liang	Soumya	Sridar	Thermodynamic modeling of LiCl-KCl-NaCl-UCl3 system facilitating molten salt electrolysis for reprocessing spent nuclear fuel
72	16:50	0:20		Jianhua	Chen	Integrated learning method based on meta-learning framework accelerates material design
73	17:10	0:20		V. B.	Rajkumar	Major revisions of the Si-Zr phase diagram
Thursday	18:00		Odyssey Dinner Cruise. Awards will be announced during the banquet.			
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Friday	**6/29/2023**	**Session 8**	**Thermodynamic Modeling, CALPHAD Database and Design Applications (II)**			
74	8:00	0:20		Karin	Frisk	CALPHAD Design of New Alloys and the Importance of the Databases
75	8:20	0:20		Colin	Stewart	ICME-Accelerated Alloy Design and Property Prediction of Novel Austenitic Steel Strengthened by Nano-precipitates
76	8:40	0:20	In-Ho Jung, Aurélie Jacob	Thomas	Avey	Iron tolerance in Mg-Ca-Zn-Mn Biomedical alloy with CALPHAD Driven Analysis

77	9:00	0:20		Manuel	Löffler	Development of thermodynamic database for ZrO2-Y2O3-HfO2-Ta2O5-system
78	9:20	0:20		Jaemin	Wang	Machine Learning for Alloy Design and Optimization of Process Conditions
79	9:40	0:20		Thomas	Matson	Construction of Phase and Defect Diagrams from a Spectral Regular Solution Model for Grain Boundary Segregation
Break	**10:00**	**0:30**	**Thermodynamic Modeling, CALPHAD Database and Design Applications (III)**			
80	10:30	0:20		Chunhui	Luo	Applications of CALPHAD in modeling microstructure in casting and thermo-mechanical processing of steels
81	10:50	0:20		Stephanie	Lippmann	Temperature gradients for materials characterization
82	11:10	0:20	Jean-Marc Joubert, Hans Jürgen Seifert	Agustin	Flores	Experimental investigation and thermodynamic assessment of the Cr–Mo–Ti system
83	11:30	0:20		Héléna	Verbeeck	Application of phase-field modeling to the recovery of Pt nanoparticles from spent automotive catalysts.
84	11:50	0:20		Wei	Xiong	Materials Design in Additive Manufacturing Using CALPHAD-based ICME Modeling with High-Throughput Experimentation
	12:10	0:10		Yu Zhong & Wei Xiong		Closing remarks
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