Conference Program of CALPHAD XLIX 2022

Sunday May 22

14:00 – 18:00	Registration	*(in Hotel Reception)*
18:00 – 21:00	Welcome Reception	*(in Event Arena)*

Venue: *Skogshem & Wijk, Lidingö*

Our Sponsors

Monday May 23 *(Event Arena)*

08:40			**OPENING**	
			Chairs:	**Malin Selleby, Anders Engström**
			Session 1:	**CALPHAD Assessment and database development**
			Chairs:	**Qing Chen, Nathalie Dupin**
09:00	O1	Bengt	Hallstedt	Hybrid Calphad DFT modelling of the Mg–Al–Ca system
09:20	O2	Erwin	Povoden-Karadeniz	Revision of precipitate modeling for applied Calphad in high-alloy steel
09:40	O3	Jonas	Lachmann	Thermodynamics in the course of Nb3Sn formation
10:00	O4	Nicolás García	Arango	Applied Calphad for the deformation-induced formation of secondary precipitates in Al-base metal microalloyed by Cu, Sc and Y
10:20	O5	Lorenzo	Fenocchio	Development of a thermodynamic database for high temperature materials
10:40				**Coffee-break** *(Café/bar)*
			Session 2:	**CALPHAD Best practice**
			Chairs:	**Zi-Kui Liu, Klaus Hack**
11:10	O6	Ji-Cheng (JC)	Zhao	Which Experimental Datasets to Trust During CALPHAD Assessments of Phase Diagrams and Diffusion Coefficients?
11:30	O7	Jean-Marc	Joubert	Estimation of fcc Al specific heat above its melting point using a reverse Neumann-Kopp approach
11:50	O8	Bo	Sundman	Calphad - the science of extrapolations
12:10	O9	Suzana G.	Fries	The materials change but not the thermodynamics
12:30				**Lunch** *(Dining)*
			Session 3:	**Structural defects and chemical inhomogeneities**
			Chairs:	**Marcel Sluiter, Benjamin Burton**
14:00	O10	Jörg	Neugebauer	Constructing defect phase diagrams from ab initio calculations and CALPHAD concepts
14:20	O11	Moritz	to Baben	Including state-of-the-art physical understanding of thermal vacancies in Calphad models
14:40	O12	Tobias	Spitaler	On the thermodynamics of binary W-Ti and its nano-crystalline stability
15:00	O13	Mira	Todorova	Using ab-initio phase diagrams to rationalize the impact of experimental preparation routes on nanoparticle impurity content
15:20				**Coffee-break** *(Café/bar)*
			Session 4:	**Oxides**
			Chairs:	**Alexander Pisch, Lina Kjellqvist**
15:50	O14	Scott James	McCormack	In-Situ Phase Diagram Determination and Symmetry Decomposition of the HfO2-Ta2O5-TiO2-Temperature System Up to 3000 °C
16:10	O15	Shivani	Gonde	Thermodynamic modelling of NASICON sub-system ZrO2-SiO2-P2O5
16:30	O16	Chancel M.	Moundounga	3rd generation modeling of the CaO-Al2O3 system
16:50	O17	Wahab	Abdul	Third-generation modelling of thermodynamic properties of cement clinkers.
18:00				**Dinner** *(Dining)*
19:30	21:30			**Poster Session** *(Event Arena)* FactSage student poster awards presented by Thermfact Ltd. and GTT Technologies

Tuesday May 24 *(Event Arena)*

			Session 5:	**Modelling and prediction of properties**
			Chairs:	**Bengt Hallstedt, Erwin Povoden-Karadeniz**
09:00	O18	Javier	Jofre	Insights on anharmonicity and self-consistency of a flexible quasi-harmonic-based approach for computational thermochemistry
09:20	O19	Li-Fang	Zhu	Melting properties from ab initio using efficient TOR-TILD approach: Applications to refractory metals V, W and V-W binary alloy
09:40	O20	Sufyan M.	Shaikh	Strategies to improve deformability of entropy stabilized refractory solid solutions
10:00	O21	Hai-Lin	Chen	CALPHAD modelling of electrical and thermal transport properties in metals and alloys
10:20	O22	Dimitra	Spathara	Study on the high temperature oxidation of single crystal Ni-based superalloys CMSX-4 and CMSX-10N
10:40				**Coffee-break** *(Café/bar)*
			Session 6:	**Additive Manufacturing**
			Chairs:	**Wei Xiong, Bartek Kaplan**
11:10	O23	Bonnie	Hagen	Using Calphad based tools to optimize alloys for Additive Manufacturing applications
11:30	O24	Karin	Frisk	Novel Alloys Designed for Laser Remelting by Computational Alloy Design
11:50	O25	Noah	Sargent	Design of Functionally Graded Steels Using CALPHAD and Experiments
12:10	O26	Chunhui	Luo	A robust thermal and microstructure modelling tool for Additive Manufacturing based on ICME approach
12:30				**Lunch** *(Dining)*
			Session 7:	**Pressure dependence**
			Chairs:	**Suzana G. Fries, Mira Todorova**
14:00	O27	Yuri	Kirshon	High-pressure high-temperature differential thermal analysis measurements in a 'Paris-Edinburgh' for solid and liquid metals
14:20	O28	Guy	Makov	Pressure dependence of binary phase diagrams: Experiments and thermodynamic modelling
14:40	O29	Byeong-Joo	Lee	Pressure dependence of thermodynamic interaction parameters for binary solid solution phases: An atomistic simulation study
15:00	O30	M. J.	Kriegel	Pressure dependent phase stabilities in the binary Ti–Fe system
15:20				**Coffee-break** *(Café/bar)*
			Session 8:	**Magnetism and elastic strain energy**
			Chairs:	**Jörg Neugebauer, Moritz to Baben**
15:50	O31	Fredrik	Haglöf	Calculation of finite temperature thermodynamic properties for metastable magnetic allotropes
16:10	O32	Tilmann	Hickel	Magneto-chemo-structural coupling during the diffusion to and phase transformation at grain boundaries in Fe-Mn alloys
16:30	O33	Qing	Chen	Modeling of Magnetic Contribution
16:50	O34	George	Kaptay	Equilibrium of strained coherent nano-particles in a solid matrix
18:00				**Dinner** *(Dining)*
20:00				**CALPHAD Board meeting** *(Sal 5)*

Wednesday May 25 (Event Arena)

			Session 9:	**Phase transformations**
			Chairs:	**Ji-Cheng (JC) Zhao, George Kaptay**
09:00	O35	Stephanie	Lippmann	Competitive solid-state reactions in multicomponent brass alloys
09:20	O36	Rutger	Slooter	Investigation of NbC proto-nuclei in steel
09:40	O37	Rainer	Schmid-Fetzer	Phase-transformation characteristics of dealloying on nanoscale
10:00	O38	Aurélie	Jacob	Exploring the formation mechanism of s phase in hyper duplex steels by in-situ experiments and computation
10:20	O39	John	Ågren	CALPHAD analysis of evaporation
10:40				**Coffee-break** *(Café/bar)*
			Session 10:	**Electronic materials**
			Chairs:	**Jean-Marc Joubert, Scott James McCormack**
11:10	O40	Andreas	Leineweber	Reconciling Crystallography, Thermodynamics and Transformation kinetics in Cu-rich NiAs/Ni2In-type Cu-Sn phases
11:30	O41	Benjamin	Burton	First principles study of the 2D Mo(S,Te)2 TMD alloy: in bulk; Adsorbed on an Al-terminated Sapphire; Between Layers of Graphene; and on Graphite.
11:50	O42	Ioana	Nuta	Gaseous phase thermodynamics for TaN thin films
12:10	O43	Silvana	Tumminello	Development of contacts for Mg2(Si,Sn)-based thermoelectric devices within a CALPHAD-based ICME framework
12:30	14:00			**Lunch** *(Dining)*
14:00	17:00			**Social Tour – Boat trip in the archipelago**
18:00				**Outdoor dinner** Sponsored by QuesTek Innovations
20:00				**Young Calphadians** *(Event Arena)* Sponsored by Sandvik Coromant

Thursday May 26 *(Event Arena)*

			Session 11:	**CALPHAD modelling for a sustainable world**
			Chairs:	**John Ågren, Sten Wessman**
09:00	O44	Jia	Qi	Experimental study and thermodynamic assessment of Li2CO3-K2CO3
09:20	O45	Xing	Fangzhou	CALPHAD-driven Design of Lithium Battery Cathodes – A Case Study in Li-Mn-O system
09:40	O46	Olga	Fabrichnaya	The development of thermodynamic database for modelling of Li recycling
10:00	O47	David	Sedmidubský	Phase equilibria in systems involving misfit layer cobaltites
10:20	O48	Sedi	Bigdeli	Towards building a computational platform for high-temperature corrosion of metallic materials using Calphad approach
10:40				**Coffee-break** *(Café/bar)*
			Session 12:	**3rd generation models**
			Chairs:	**Bo Sundman, Richard Otis**
11:10	O49	Zhangting	He	Third generation of Calphad: from unary to higher-order systems
11:30	O50	Alexander	Walnsch	Development of a third generation CalPhaD database of Fe–Mn–Ti by applying advanced sublattice models for complex crystal structures
11:50	O51	Liangyan	Hao	Application of the third generation CALPHAD data and models in two binary systems: Ga-Ni and Mn-Ni
12:10	O52	Alexander	Pisch	3rd generation modeling of the thermodynamic properties of oxides
12:30				**Lunch** *(Dining)*
			Session 13:	**Data mining/ML and uncertainty quantification**
			Chairs:	**Byeong-Joo Lee, Sedi Bigdeli**
14:00	O53	Jean-Claude	Crivello	Multi-component sigma-phase database built with the help of high-throughput DFT calculation and supervised machine learning
14:20	O54	Adam	Krajewski	Structure-Informed Prediction of Formation Energy and New Material Discovery Tools
14:40	O55	Qi-Jun	Hong	Design of high-melting-temperature materials via first principles and deep learning
15:00	O56	Brandon	Bocklund	A general approach for computing the residuals between CALPHAD models and phase diagram data
15:20				**Coffee-break** *(Café/bar)*
			Session: 14	**Process simulation and life-time prediction**
			Chairs:	**Rainer Schmid-Fetzer, Gabriele Cacciamani**
15:50	O57	Willem	Roos	Geometric Acceleration of Complex Equilibrium Calculations for Integration in High-temperature Models
16:10	O58	André	Costa e Silva	Application of a Computational Thermodynamics “Effective Equilibrium Reaction Zone” (EERZ) Model to the Secondary Refining of Steels
16:30	O59	Werner	Verdier	Coupling a grand potential ternary phase field model to the thermodynamic landscape of the Na2O-SiO2-MoO3 nuclear glass
16:50	O60	Clément	Introïni	On the coupling of a CALPHAD database with a phase-field modeling of incipient melting and oxygen transport in nuclear fuel during power transients
19:00				**Aperitif** *(Café/bar & Foajé)*
20:00				**Conference banquet** *(Event Arena)* *Sponsored by Jernkontoret*

Friday May 27 *(Wijken)*

			Session 15:	**High Entropy Alloys**
			Chairs:	**Hai-Lin Chen, Bonnie Hagen**
09:00	O61	Ahmadreza	Riyahi khorasgani	Incorporation of CALPHAD method into continuum modelling of interdiffusion in HEAs
09:20	O62	Huahai	Mao	Thermodynamic database for high entropy alloys and its application on non-equilibrium phase transformations
09:40	O63	Alvise Miotti	Bettanini	Combined computational and experimental alloy design of High Entropy Alloys processed by additive manufacturing
10:00	O64	Marcel	Sluiter	Hydrogen in TiZrHfVNb high entropy alloys
10:20	O65	Wei	Chen	Data-Driven Design of High-entropy Alloys
10:40				**Coffee-break** *(Café/bar)*
			Session 16:	**Thermodynamic theory, modelling and application**
			Chairs:	**Andre Costa e Silva, Huahai Mao**
11:10	O66	Zi-Kui	Liu	Zentropy
11:30	O67	Maryam	Kazemzadeh-Atoufi	Carburization and oxidation calculations of a Ni-Cr-Fe based high-temperature austenitic alloy and nucleation of austenite at the carbide transition front
11:50	O68	Haoxue	Han	A high throughput thermodynamic calculation workflow for ternary phase diagram: beyond three-dimensional reconstruction
12:10	O69	Wei	Xiong	Fundamental Issues Identified in Thermodynamic Database Development for Molten Salt Systems
12:30				**Closing by Malin Selleby**
12:30	14:00			**Lunch** *(Dining)*