Oral presentations

Monday, June 12, 2017

08:45-09:00	**Opening**	
		Keynote lecture, chair: J.-C. Crivello
09:00-09:40	**K1**	**Software tools for high-throughput CALPHAD from first-principles data** van de Walle Axel

Session: Configurational thermodynamics
Chairs: G. Kaptay - B. Sundman

09:40-09:55	**O1**	First Principles Calculation of the WS_2-WTe_2, Phase Diagram Burton Benjamin
09:55-10:10	**O2**	Stability of $NdFe_{12}$(N) Series Compounds: A First-principles Study Saengdeejing Arkapol, Chen Ying
10:10-10:25	**O3**	Configurational thermodynamics of C in bcc Fe: a combined computational study Yan Jiayi, Ruban Andrei
10:25-10:40	**O4**	Configurational energy of formation of alloys: Ising models vs the Cluster Expansion Sanchez Juan
10:40-11:10	**Coffee Break**	

Session: First principles and high-throughput
Chairs: A. Kroupa - B.-J. Lee

11:10-11:25	**O5**	Alloying and Phase Stability in MAX Phases: A High-throughput Cluster Expansion Approach Arróyave Raymundo, Talapatra Anjana, Duong Thien, Son Woongrak, Prehn Evan, Gao Huilio, Radovic Miladin
11:25-11:40	**O6**	Comparison of calculated and experimental values of enthalpies of formation of intermetallic compounds. Colinet Catherine, Tedenac Jean-Claude
11:40-11:55	**O7**	Nickel incorporation in Ti_2AlC ceramic Lu Chengjie, Zhang Jie, Hug Gilles
11:55-12:10	**O8**	Ground state predictions for sulfide electrolytes likubo Satoshi, Shimoyama Koichi, Kawano Shoya, Fujii Masafumi, Matsushita Masafumi, Shinmei Toru, Ohtani Hiroshi
12:10-12:25	**O9**	A New Methodology for High-throughput Screening of Composition-Microstructure-Micromechanical Properties Relationships Cui Yuwen, Guanglong Xu
12:25-14:00	**Lunch**	

Session: Thermo-kinetics and diffusion
Chairs: J. Ågren - A. Costa e Silva

14:00-14:15	**O10**	Impacts of thermodynamic and kinetic model parameterisation on precipitation simulations - Case study of NbC precipitation in microalloyed steel Povoden-Karadeniz Erwin, Kozeschnik E.
14:15-14:30	**O11**	Thermo-kinetic modeling for the growth/dissolution of α slabs and lamellae in Ti-55531 under continuous heating condition Chen Fuwen, Xu Guanglong, Zhang Xiaoyong, Zhou Kechao
14:30-14:45	**O12**	Overcoming the Diffusion Bottleneck: Effect of Alloying Elements on Phase Transformations and Carbide Dissolution in Martensitic Stainless Steels Miotti Bettanini Alvise, Delannay Laurent, Pardoen Thomas, Mithieux Jean-Denis, Badinier Guillaume, Pascal Jacques
14:45-15:00	**O13**	Temperature Dependence of Diffusivities from a Single Experiment - Experimental Technique and Evaluation Method Engelhardt Hannes, Rettenmayr Markus
15:00-15:15	**O14**	Diffusivities and Atomic Mobilities in fcc Cu-Ni-Sn Alloys Liu Yuling, Liu Dandan, Du Yong, Liu Shuhong
15:15-15:30	**O15**	Analytical model with interaction between species for growth and dissolution of precipitates Gandin Charles-André, Guillemot Gildas
15:30-18:00	**Poster session A, chair: M. Perrut**	

Session: Phase field and molecular dynamics
Chairs: A. Khvan - A. Gheribi

18:00-18:15	**O16**	Quantitative phase-field simulation of microstructure evolution in Ni-Al alloys during entire preparation process and its linking to mechanical property Zhang Lijun, Cao Dongjia, Lin Yan
18:15-18:30	**O17**	Microstructure evolution during melting of single crystal superalloy: A combined experimental and computational study Warnken Nils, Chen Xu, Slater Carl
18:30-18:45	**O18**	Matching time and spatial resolutions of rapid solidification: Dynamic TEM experiments coupled to CALPHAD-informed phase-field simulations Perron Aurélien, Roehling John, Turchi Patrice, Fattebert Jean-Luc, Mckeown Joseph
18:45-19:00	**O19**	Glass Transition Temperature and Phase Diagrams of Butadiene Rubber and Styrene Butadiene Rubber: Molecular Dynamics Simulation Lee Hyuck Mo, Ryu Myung Shin, Kim Hyoung Gyu, Bang K.
19:00-20:00	**Free Time**	
20:00-21:00	**Dinner**	
21:00-23:00	**Evening session: Young Calphadian Meeting, chair: S. Gossé OR free poster viewing**	
-	with the participation of C. Colinet, B. Sundman and B.-J. Lee	

Tuesday, June 13, 2017

Keynote lecture, chair: C. Guéneau

09:00-09:40 **K2** **Ab initio based multiscale modelling in physical metallurgy**
Willaime François, Lüthi B., Marinica M.C., Ventelon L., Rodney D.

Session: First principles and nanos
Chairs: P. Chartrand - S. Nishitani

09:40-09:55 **O20** Phase stability and chemical composition of nanoprecipitates: A first principles study for the example of kappa carbides
Hickel Tilmann, Dey Poulumi, Dutta Biswanath, Friák Martin, Neugebauer Jörg

09:55-10:10 **O21** The size-dependent phase diagram form Ni-based systems by combination of CALPHAD and ab initio methods
Kroupa Ales, Kana Tomas, Vykoukal Vit, Zemanova Adela, Svoboda Milan, Sob Mojmír, Pinkas Jiri

10:10-10:25 **O22** Constructing an As-Ga-In-Sn thermodynamic database for modelling the growth of InAs, GaAs and $In_xGa_{1-x}As$ nanostructures
Ghasemi Masoomeh, Johansson Jonas

10:25-10:40 **O23** First-principles Calculation Assisted Thermodynamic Modeling of B-Ta and B-C-Ta System
Xuemei Ouyang

10:40-11:10 **Coffee Break**

Session: Interface and thin films
Chairs: R. Arróyave - Y. Du

11:10-11:25 **O24** Interface energy at limit radius in metallic system
Nishitani Shigeto

11:25-11:40 **O25** Temperature and concentration dependent solid/liquid interfacial energies
Lippmann Stephanie, Jung In-Ho, Paliwal Manas, Rettenmayr Markus

11:40-11:55 **O26** Modeling of metastable phase formation diagrams for sputtered thin films
Chang Keke, Music Denis, To Baben Moritz, Lange Dennis, Bolvardi Hamid, Schneider Jochen

11:55-12:10 **O27** Calculation of phase diagrams with epitaxial orientations in Co-based binary alloy thin films
Lu Yong

12:10-12:25 **O28** Thermodynamic study on grain boundary segregation
Ohtani Hiroshi, Enoki Masanori, Higashide Yusuke

12:25-14:00 **Lunch**

Session: Assessment: carbides and metallic systems
Chairs: B. Lindhal - P. Turchi

14:00-14:15	**O29**	A new thermodynamic database of Ti(C,N)-based cermets and its application to the control of grain growth Du Yong, Zhang Cong
14:15-14:30	**O30**	Thermodynamic assessment of the C-Zr system Davey Theresa, Mellan Thomas, Fries Suzana, Finnis Michael
14:30-14:45	**O31**	From ternary experiments back to binary modeling: Li-Si-C example Schmid-Fetzer Rainer, Liang Songmao, Drüe Martin, Kozlov Artem, Rettenmayr Markus
14:45-15:00	**O32**	Modelling the Gibbs energy of Ag-Ni, Ag-Ge and Ag-Ge-Ni by calphad approach Rajkumar V.B, Chen Sinn-Wen
15:00-15:15	**O33**	Thermodynamic modelling of Long Periodic Stacking Ordered (LPSO) phases in Mg-Gd-Al ternary system Kim Hongyeun, Ross Austin, Shang Shunli, Wang Yi, Kecskes Laszlo, Darling Kristopher, Liu Zi-Kui
15:15-15:30	**O34**	Phase equilibria of Pb-Sb-Se-Sn quaternary system Chen Sinn-Wen, Chang Jui-Shen
15:30-18:00	**Poster session B, chair: M. Perrut**	

Session: Assessment: oxides
Chairs: E. Povoden-Karadeniz - M. Selleby

18:00-18:15	**O35**	Phase relations in the ZrO_2-TiO_2-Al_2O_3 system: experimental study and thermodynamic assessment Fabrichnaya Olga, Ilatovskaya Mariia, Savinykh G.
18:15-18:30	**O36**	Thermodynamic properties of oxide compounds estimated from polyhedron method Jung In-Ho, Moosavi-Khoonsari Elmira, Wu Ting
18:30-18:45	**O37**	Integrated experimental and thermodynamic modelling research on the multicomponent Pb-Cu-Fe-Zn-Ca-Si-O system Shevchenko Maksym, Shishin Denis, Jak Evgueni
18:45-19:00	**O38**	Thermodynamic investigation of the Cr-O-U and Cr-O-Zr systems Lindahl Bonnie, Alpettaz Thierry, Bonnaillie Patrick, Brackx Emmanuelle, Chatain Sylvie, Domenger Renaud, Gossé Stéphane, Poissonnet Sylvie, Guéneau Christine
19:00-20:00	**Free Time**	
20:00-21:00	**Dinner**	
-	**Evening session: Computer session, chair: A. Pisch OR free poster viewing**	
21:00-21:30	**C1**	What is New in Thermo-Calc Chen Qing
21:30-22:00	**C2**	Demonstration of Pandat software Chen Shuanglin and Schmid-Fetzer Rainer
22:00-22:30	**C3**	Fact-Sage Jung In-Ho

Wednesday, June 14, 2017

Keynote lecture, chair: I. Nuta

09:00-09:40 **K3** **Experimental Thermodynamics of Nuclear Materials**
Konings R.J.M., Beneš O., Capelli E., Manara D., Popa K., Pavlov T., Vlahovic L.

Session: Experimental measurements I
Chairs: S. Lippman - B. Oudot

09:40-09:55 **O39** Standard Enthalpies of Formation of Select Cu_2YZ Compounds
Nash Philip, Hasier John, Hawgood Mary, Kim George, Chen Wei

09:55-10:10 **O40** Calorimetric determination of the formation enthalpy of ZnSb
Benigni Pierre, Berche Alexandre, Pothin Romain, Adenot Aurélien, Mikaelian Georges, Ayral Rose-Marie, Jund Philippe, Rogez Jacques

10:10-10:25 **O41** Gaseous phase thermodynamics of organometallics: a TaN-precursor study
Nuta Ioana, Blanquet Elisabeth, Artaud Laurent, Collas Hervé, Chatillon Christian

10:25-10:40 **O42** Thermodynamic Vaporization Studies of Lead Oxide and Sodium Oxide with Knudsen Effusion Mass Spectrometry
Kobertz Dietmar

10:40-11:10 **Coffee Break**

Session: Experimental measurements II
Chairs: P. Benigni - P. Nash

11:10-11:25 **O43** A container-less electrochemical method to evaluate the thermodynamic properties of molten oxides and liquid alloys
Allanore Antoine, Nakanishi Bradley

11:25-11:40 **O44** On the Quaternary System Ce-Ni-Zn-B
Rogl Peter, Failamani Fainan, Podloucky Raimund, Malik Zahida, Bursik Jiri, Grytsiv Andrij, Bauer Ernst

11:40-11:55 **O45** Determination of phase equilibria in Fe-C-Mn-Al alloys for 3rd generation duplex steels
Mestrallet Aurore, Antoni-Zdziobek Annie, Emo Jonathan, Maugis Philippe, Hallstedt Bengt

11:55-12:10 **O46** Alloy phase stability under electric currents
Lin Shih-Kang, Liu Yu-Chen

12:10-19:00 **Excursion**

19:00-20:00 **Free Time**

20:00-23:00 **Conference Banquet**

Thursday, June 15, 2017

Keynote lecture, chair: J.-M. Joubert

09:00-09:40 **K4** **Thermodynamic and physical-property models for the production of primary aluminium**
Chartrand Patrice, Gheribi Aimen Ernest, Wang K., Ouzilleau P., Robelin Christian

Session: Liquids and salts
Chairs: C. Colinet - O. Fabrichnaya

09:40-09:55 **O47** Uncertainty quantification in ternary interpolation methods for thermodynamic properties of liquid alloys
Beyers Lesley, Van Den Bulck Amy, Wollants Patrick

09:55-10:10 **O48** Thermodynamic modeling and experimental investigations in the H_2O - HNO_3 - $Sm(NO_3)_3$ - $Eu(NO_3)_3$ - $(C_4H_9O)_3PO$ system
Kovalenko Nikita, Maksimov Aleksey, Arkhipin Anatoly, Voronin Gennady

10:10-10:25 **O49** Phosphoric acid and sodium phosphate: Extending the limit of aqueous electrolyte modelling
Wang Peiming

10:25-10:40 **O50** DFT/CALPHAD mixed method for the prediction of the thermal transport properties within aluminium electrolysis cells
Gheribi Aimen Ernest, Chartrand Patrice

10:40-11:10 **Coffee Break**

Session: Assessment: metallic systems
Chairs: M. Kurata - A. Jacob

11:10-11:25 **O51** Engineering applications of CALPHAD - some examples
Ågren John

11:25-11:40 **O52** The formation of magnesiowustite in steelmaking slag evaluated experimentally and via computational thermodynamics
Costa e Silva Andre, Vieira Alan, Martins Antonio Augusto, Batista Rafaela, Avillez Roberto

11:40-11:55 **O53** Thermodynamic features of the Al-Mo and Al-Mo-Ti systems
Kriegel Mario, Klemm Volker, Fabrichnaya Olga, Freudenberger Jens, Leineweber Andreas

11:55-12:10 **O54** New assessment of the Al-Fe system
Zienert Tilo, Fabrichnaya Olga

12:10-12:25 **O55** A thermodynamic database for cast iron
Hallstedt Bengt

12:25-14:00 **Lunch**

Keynote lecture, chair: C. Toffolon Masclet

14:00-14:40	**K5**	**On the 3rd Generation of Thermodynamic Databases** Selleby Malin

Session: 3rd generation and models
Chairs: C.-A. Gandin - B. Burton

14:40-14:55	**O56**	Experimental study and modeling of thermodynamic properties of the Ag-Cu system for the third generation of thermodynamic databases Phiri Albina, Khvan Alexandra, Dinsdale Alan
14:55-15:10	**O57**	On the temperature dependence of excess Gibbs energy of solutions Kaptay George
15:10-15:25	**O58**	Modelling thermal vacancies within the CALPHAD approach Liu Zi-Kui, Guan Pin-Wen
15:25-15:40	**O59**	Thermodynamic descriptions of pure Sn, Pb, Bi and Bi-Sn system from 0K using two state model for the liquid phase. Khvan Alexandra, Dinsdale Alan, Phiri Albina
15:40-15:55	**O60**	About the limits of applicability of the Alkemade theorem for the construction of ternary liquidus surfaces Stein Frank, He Cuiyun
15:55-16:10	**O61**	The Calphad Method - the Scientific use of Metastability Sundman Bo
16:10-16:45	**Coffee Break**	

Session: HEA and thermodynamic modelling
Chairs: N. David - R. Schmid-Fetzer

16:45-17:00	**O62**	Understanding Physical Metallurgy and Computational Design of High Entropy Alloys: Atomistic Simulation and CALPHAD Lee Byeong-Joo, Choi Won-Mi
17:00-17:15	**O63**	The fcc solid solution stability in multi-component system :towards high entropy alloys design Bracq Guillaume, Laurent-Brocq Mathilde, Perrière Loïc, Pires Rémy, Crivello Jean-Claude, Joubert Jean-Marc, Guillot Ivan
17:15-17:30	**O64**	A Constraint Satisfaction Problem Approach to High-Entropy Alloy Design Abu-Odeh Anas, Chaudhary Nayan, Gibbons Sean, Galvan Edgar, Kirk Tanner, Mao Huahai, Malak Richard, Arróyave Raymundo
17:30-17:45	**O65**	Phase stabilities of Ti materials with a focus on the thermodynamic modelling of metastable microstates Marker Cassie, Shang Shunli, Zhao Ji-Cheng, Liu Zi-Kui
17:45-18:00	**O66**	Crystal structure relations among variants of the ω phase in titanium alloys and their modeling Chen Hai-Lin
18:00-18:15	**O67**	Characterizing uncertainty of CALPHAD assessment. The Au-Pd case Kuznetsov Victor
18:15-18:30	**O68**	Thermodynamic modelling of Cr-Fe-Nb-Sn-Zr system Lafaye Paul, Crivello Jean-Claude, Toffolon-Masclet Caroline, Joubert Jean-Marc
18:30-18:45	**O69**	A New Approach of the CEF applied to the sigma phase modeling : Application to the thermodynamic re-assessment of the Nb-Al system using new experimental data. Fiorani Jean-Marc, Araújo Pinto Da Silva Antonio Augusto, Carvalho Coelho Gilberto, Nunes Carlos, David Nicolas, Vilasi Michel
18:45-19:00	**O70**	Thermodynamic study on microstructure evolution during aging process in the Al-Cu binary alloy Yabe Takahiro, Shibahara Shohei, Enoki Masanori, Ohtani Hiroshi
19:00-20:00	**Free Time**	
20:00-21:00	**Dinner**	

Friday, June 16, 2017

Keynote lecture, chair: A. Antoni Zdziobek

09:00-09:40 **K6** **Calphad Study of Planetary Condensation**
Saxena Surendra

Session: Applications
Chairs: K. Frisk - F. Stein

09:40-09:55 **O71** Phase diagrams of alloys under pressure
Makov Guy, Emuna Moran, Yahel Eyal, Greenberg Yaron

09:55-10:10 **O72** Thermodynamic description of the lithium manganese oxide as cathode materials for lithium-ion batteries
Zhang Weibin, Cupid Damian, Seifert Hans

10:10-10:25 **O73** Thermodynamics on Developing Earthquake Resisting Thermodynamics on Developing Earthquake Resisting
Lee Joonho, Hwang Byoungchul, Shim Jae-Hyeok, Lee Myoung-Gyu, Jung Jun-Ho, Kim Bo-Sung, Won Sung-Bin

10:25-10:40 **O74** A CALPHAD approach to modelling of slag viscosities
Hack Klaus, Yakshenshikh Elena, Wu Guixuan, Mueller Michael, Jantzen Tatjana

10:40-11:10 **Coffee Break**

Session: Nuclear materials, catalysts and cemented carbides
Chairs: S. Gossé - A. Perron

11:10-11:25 **O75** Thermodynamics of Actinide Alloys in the upcoming New Edition of the Pu Handbook
Turchi Patrice, Perron Aurélien, Timofeeva Lidia, Clark David, Hanrahan Robert

11:25-11:40 **O76** CALPHAD approach: a complementary way to determine the corrosion path way of PuAl alloys stabilized in delta-phase
Oudot Benoit, Ravat Brice, Jolly Lionel, Perron Aurélien, Turchi Patrice, Guéneau Christine, Delaunay Francois

11:40-11:55 **O77** PdZn Intermetallic compound: A pseudoelement of Cu for catalysis
Tsai An Pang, Kameoka Satoshi, Shimoda Masahiko, Ishii Yasushi

11:55-12:10 **O78** Design of grain growth inhibitors and analysis of mechanical properties in ultra-fine WC-10Co cemented carbides based on thermodynamic calculations
Haixia Tian, Peng Yingbiao, Du Yong

12:10-12:25 **O79** Thermodynamic and Kinetic Modeling Applied to Hardmetals
Frisk Karin

12:25-12:40 **Closing**

12:40-14:00 **Lunch**