Monday (Morning), May 23
Ab Initio

08:20	**Welcome remarks**
	Chairs Dr. Patrice Turchi Prof. Fernando Rizzo
[O1] 08:50	*J.M. Sanchez* The Cluster Expansion Method: First Principles or Phenomenology?
[O2] 09:20	*Jörg Neugebauer, Blazej Grabowski, Albert Glensk, and Tilmann Hickel* Accuracy and limitations of ab initio approaches in predicting free energies for binaries and unstable phases
[O3] 09:50	*Helena Maria Petrilli, Ney Sodré, Pablo Guillermo Gonzales-Ormeño, Claudio Geraldo Schon* Ab-initio calculation of the bcc order/disorder relations in the Al - Cr - Fe (Aluminum - Chromium - Iron) system
[O4] 10:10	*Benjamin Burton, A. van de Walle* First Principles Phase Diagram Calculations for the systems: SiC-AlN; SiC-GaN; SiC-InN; and ZrO_X (0 < X < 1)
[O5] 10:30	*Gilles Hug, Philippe Jund, Romain Viennois, Catherine Colinet, Jean-Claude Tédenac* Ab initio modeling in the Mg-Si system
10:50	**Coffee-break**
	Chairs Prof. Catherine Colinet Prof. Igor A. Abrikosov
[O6] 11:15	*Tetsuo Mohri* Progress of theoretical study of alloy phase equilibria based on Cluster Variation Method
[O7] 11:45	*Jan Vřesťál, Jana Pavlů* Laves phases in the Hf-V and V-Zr systems: Stability analysis using ab initio data and phase diagrams
[O8] 12:05	*J. Pavlů, J. Vřešťál, M. Šob* Energetics and magnetism of Mo-based sigma phases
[O9] 12:25	*Susana Ramos de Debiaggi, Críspulo Deluque Toro, Gabriela F. Cabeza, Armando Fernández Guillermet* Thermodynamic properties of M-In-Sn (M = Cu, Ni) intermetallics: Ab initio database and systematics
[O10] 12:45	*Anjali Talekar, Dhanesh Chandra* Ternary Phase Diagrams for Plastic Crystal Energy Storage Materials - Computational and Experimental Approach
13:05	**Lunch**

Monday (Afternoon), May 23

	Chairs Prof. Jan Vrestal Prof. Cláudio G. Schon
[O11] 14:30	*Igor Abrikosov, Björn Alling, Marcus Ekholm, Hans Lind, Ferenc Tasnadi* Configurational thermodynamics of multicomponent complex alloy systems from first-principles theory
[O12] 15:00	*S.R.Nishitani, K. Togase, Y. Ohno, Y. Tokumoto, and I. Yonenaga* First principles calculations of stacking fault energy of P doped Si crystal
[O13] 15:20	*Sung Hoon Lee, Zi-Kui Liu* Computational and experimental investigations of defects and stability of (La1-xCax)$FeO_{3-\delta}$ perovskites
[O14] 15:40	*Torsten Markus, Jens Emmerlich, Denis Music, Li Yang* Phase stability and thermomechanical properties of LSCF and BSCF perovskites
[O15] 16:00	*Jianchuan Wang, Yong Du, Honghui Xu, Lixian Sun, Zi-Kui Liu* Formation and migration of native defects in complex hydrides
[O16] 16:20	*Byeong-Joo Lee, Je-Wook Jang, Kyu-Seok Han, Chan-Hee Han* A comparative analysis of the effect of particle pinning and solute segregation on the inhibition of grain boundary movement
16:40	**Coffee-break**
	Chairs Prof. Tetsuo Mohri Prof. Byeong-Joo Lee
[O17] 17:05	*Patrice E. A. Turchi, Alexander I. Landa* Actinide alloys and their challenges
[O18] 17:35	*Catherine Colinet, Jean-Claude Tedenac* Structural stability of the ternary compounds Mo5SiB2 and Nb_5SiB_2
[O19] 18:05	*Jean-Marc Joubert, Aurore Mascaro, Jean-Claude Crivello, Caroline Toffolon-Masclet* Ab-initio calculations of Er-H compounds: application to the modelling of the phase diagram
[O20] 18:25	*J.-C. Crivello, M. Palumbo, T. Hammerschmidt, S.G. Fries, J.-M. Joubert* Calculating heats of formation using DFT: guidelines for the study of TCP phases
[O21] 18:45	*Wei Xiong, Pavel Korzhavyi, Qing Chen, Malin Selleby* Bridging ab initio and CALPHAD by a robust magnetic model
19:05	**Dinner**
20:30 22:30	**Poster Session**

Tuesday (Morning), May 24
The CALPHAD Method, and Assessments

	Chairs Dr. Larry Kaufman Dr. Suzana Fries
[O22] 08:30	*John Ågren* Calphad - what did we hope for, what did we get - where do we go?
[O23] 09:00	*Reza Naraghi, Malin Selleby* Reassessment of the thermodynamic description of the Fe-C system
[O24] 09:20	*D. Chandra, A. Talekar, J. Lamb,W-M Chien, D. Phanon, Nicolas Penin, Radovan Černý, Klaus Yvon, J-C Crivello, M. Latroche, and M. Gupta* Ternary Phase Diagram of Li-N-H Complex Hydrides for Hydrogen Storage Systems
[O25] 09:40	*Chonghe Li* Thermodynamic Assessment of V_2O_3-TiO_2 System
[O26] 10:00	*F. Stein, M. Palm, S. Voß, C. He, O. Dovbenko and O. Prymak* Experimental investigations of phases, phase equilibria, and melting behaviour in the systems Fe-Al-Nb and Co-Al-Nb and their terminal binary systems
[O27] 10:20	*Hang Wang, Nils Warnken, Roger C. Reed* Phase Field Simulation on beta/alpha transformation in TiAlV system coupled with CALPHAD assessment
10:40	**Coffee-break**
	Chairs Prof. John Ågren Dr. Antonio Sérgio Fonseca
[O28] 11:05	*Larry Kaufman* Computation materials design
[O29] 11:35	*E. Povoden-Karadeniz, E. Eidenberger, P. Lang, H. Leitner, E. Kozeschnik* Thermodynamics of the Fe-Co-Mo system and modeling of early precipitation in Fe-25 at.% Co-9 at.% Mo alloy
[O30] 11:55	*Mehdi Hosseinifar* Experimental investigation and thermodynamic optimization of the Al-Mg-Nd system
[O31] 12:15	*E. Povoden-Karadeniz, P. Warczok, P. Lang, A. Falahati, M.R. Ahmadi, E. Kozeschnik* Thermodynamic modeling of metastable phases in Al-Cu-Fe-Mg-Mn-Si and applications to precipitation kinetics simulations
[O32] 12:35	*Peng Zhou, Senlin Cui, Dandan Liu, Lijun Zhang, Yong Du, Wanqi Jie* Assessment of the atomic mobilities for Fcc_a1 and Bcc_A2 Cu-Fe-Zn alloys
13:00	**Lunch**

Tuesday (Afternoon), May 24

	Chairs Dr. Bo Sundman Dr. Ursula R. Kattner
[O33] 14:30	*K. Ishida, T. Omori* New Co-base Superalloys - Phase Equilibria and Applications
[O34] 15:00	*M. Palumbo, S. G. Fries, T. Hickel, A. Dal Corso, M. H. G. Jacobs, U. R. Kattner, B. Sundman* The challenge of covering thermodynamic properties not only at high temperature but also at low temperature: a progress report
[O35] 15:20	*Dmitri V. Malakhov* Non-statistical thermodynamic optimization: an irrelevant topic or a useful approach?
[O36] 15:40	*Patrice Berthod, Lionel Aranda, Ophélie Hestin, Elise Souaillat, Moussa Ba, Ahmed Dia* Experimental and thermodynamic study of ternary Ni-30Cr-xC and Co-30Cr-yC carbon-rich alloys with x and y varying from 2.5 to 5.0 wt.%
[O37] 16:00	*Dominika Jendrzejczyk-Handzlik, Wojciech Gierlotka, Krzysztof Fitzner* Thermodynamic properties and phase equilibria in gold-antimony-tin system determined from E.M.F., Calorimetric, and dta/dsc methods
[O38] 16:20	*Olga Fabrichnaya, Hans J Seifert* Experimental study and thermodynamic modelling of phase relations in the ZrO_2-Sm_2O_3-Y_2O_3 and Sm_2O_3-Y_2O_3-Al_2O_3 systems
16:40	**Coffee-break**
	Chairs Prof. Dr. Rainer Schmid-Fetzer Prof. Roberto R. de Avillez
[O39] 17:00	*Suzana G. Fries* The role of CALPHAD in the Science of Materials
[O40] 17:30	*Yun Hwan Jo, Inyu Jung and Hyuck Mo Lee* Synthesis of Size and Composition Controlled Sn-xCu Nanoparticles: Effect on the Phase Diagram and Application to Highly Conductive Ink
[O41] 17:50	*In-Ho Jung, Marie-Aline Van Ende, Hanshin Choi, Taek-Soo Kim* Thermodynamic Database Development of the Nd-Fe-B-Mg System for the Nd-Fe-B Magnet Scrap Recycling Process
[O42] 18:10	*Shihuai Zhou, R.E. Napolitano* Nonequilibrium phase transformation calculation with Energetics
[O43] 18:30	*Biao Hu, Honghui Xu, Shuhong Liu, Yong Du, Cuiyun He, Chunsheng Sha, Wenqing Zhang, Yingbiao Peng, Dongdong Zhao and Yiwei Li* Experimental investigation and thermodynamic calculation of the Mn-Ni-Si System
[O44] 18:50	*Atta Ullah Khan, Pavel Broz, Haiyang Niu, Xingqiu Chen, Peter Rogl* The Phase Diagrams Ta-V-{Si,Ge}
19:10	**Dinner**
20:30 22:30	**Poster Session**

Wednesday (Morning), May 25
Applications - Energy

	Chairs Dr. Christine Gueneau Prof. Bo Sundman
[O45] 08:30	*Rogl Peter Franz, Noel Henri* The Phase Diagram Basis U - M -Si for LEU fuels; M=Al, Sc to Pt
[O46] 09:00	*Jeong-Yong Park, Hyun-Gil Kim, Byung-Kwon Choi, Sang-Yoon Park, Yang-Il Jung, Dong-Jun Park* Experimental study on the microstructure factors controlling the corrosion behavior of Zr alloys
[O47] 09:20	*C. Toffolon-Masclet, C. Desgranges, B. Mazères, D. Monceau* Simulation of Oxide Dissolution in Zr Alloys : Comparison between Numerical EKINOX Code and DICTRA Calculations
[O48] 09:40	*O. Beneš, R. J. M. Konings, D. Staicu* Physico-chemical properties investigation of plutonium
[O49] 10:00	*M. Beilmann, O. Benes, R. Konings* Thermodynamic assessment of a Molten Salt Reactor fuel
[O50] 10:20	*X.J. Liu, C.P. Wang* The thermodynamic database of nuclear material system
10:40	**Coffee-break**
	Chairs Dr. Ales Kroupa Prof. Kiyohito Ishida
[O51] 11:05	*Gueneau Christine, Gotcu Petronela, Benes Ondrej, Sundman Bo, Dupin Nathalie, Konings R.J.M.* Thermodynamic modelling of oxide fuels containing minor actinides (U, Pu, Am, Np)$O_{2\pm x}$
[O52] 11:35	*Ligang Zhang, Patrick J. Masset* Investigation in the CaO-SiO_2-M_2O (M = Na, K) system
[O53] 11:55	*Marc A. Duchesne, Robin W. Hughes, Dennis Y. Lu, David McCalden, Arturo Macchi, Edward J. Anthony* Application of FactSage for the Study of Slagging In Entrained-Flow Gasifiers
[O54] 12:15	*Patrick Masset, Cuiping Guo* Evaluation of the thermodynamic properties of the gas phase involved in gasification processes
[O55] 12:35	*Jean-Christophe Dumas, Jean-Paul Piron, Chantal Martial* Evaluation of the Chemical Composition of Irradiated Mixed Carbide Fuel
13:00	**Lunch**
14:30	**Conference Excursion: Visit to Fort São João in Rio de Janeiro; Visit to Sugar Loaf**
20:00 22:30	**Conference Dinner: PORCÃO Rio's**

Thursday (Morning), May 26
Applications - Steel, Superalloys, Oxides

	Chairs Prof. Andre Costa e Silva Prof. Malin Selleby
[O56] 08:30	*Tooru Matsumiya* Applications of CALPHAD in Steelmaking and Future Scope
[O57] 09:00	*André Schneider* Application of the CALPHAD method for ferritic boiler steels
[O58] 09:20	*Carlos Cicutti, Constantino Capurro* Development of a model to predict inclusions composition in steels deoxidized with aluminum, silicon and manganese
[O59] 09:40	*Bernd Böttger* Phase-Field Modelling of Technical Alloy Systems
[O60] 10:00	*T. Gómez-Acebo, F. Castro* Diffusion in Fe-Ni PM alloys: microstructure and DICTRA simulations
[O61] 10:20	*Philippe Schaffnit, Juliane Mentz, Joachim Konrad* Simulation of an Industrial Solidification Process by Coupling CALPHAD and Phase-Field
10:40	**Coffee-break**
	Chairs Prof. Dr. Jorg Neugebauer Prof. Dr. Herbert Ipser
[O62] 11:05	*Malin Selleby* How applications drive thermodynamics towards fundamental considerations
[O63] 11:35	*Henrik Strandlund, Susanne Norgren* Applications of CALPHAD in Cemented carbide development
[O64] 11:55	*B. Jansson, J. M. Ullbrand, F. Tasnádi, L. Hultman, and M. Odén* A multi scale modeling approach for transition metal nitride alloy coatings
[O65] 12:15	*Qing Chen* Challenges of Precipitation Kinetic Modelling. I. Study on Growth Rate Models
[O66] 12:35	*Ikuo Ohnuma, Shota Shimenouchi, Toshihiro Omori, Ryosuke Kainuma, Kiyohito Ishida* Phase Equilibria at Low Temperatures (< 600 °C) and Thermodynamic Evaluation in the Fe-base Binary Systems
13:00	**Lunch**

Thursday (Afternoon), May 26

	Chairs Dr. Alan J. Ardell Prof. Dr. Adolf Mikula
[O67] 14:30	*Bo Sundman, Christine Gueneau, Nathalie Dupin* Thermodynamic modelling of defects in U-Pu-O-C
[O68] 15:00	*Antonio J Ramirez, Jimy Unfried S* Design of a Ductility-Dip Cracking Resistant Ni-Cr-Fe Alloy
[O69] 15:20	*Joo Hyun Park* Applications of Computational Thermodynamics on the Fundamental Research on the Complex Metal-Oxide Systems
[O70] 15:40	*Christian Robelin, Patrice Chartrand* Overview of the Molten Chlorides, Fluorides and Chloro-fluorides Databases of the FactSage Thermochemical Software
[O71] 16:00	*Patrice Chartrand, Christian Robelin, Matthias Heyrman, Nagendra Tripathi* The Cryolite Database for the Hall-Heroult Alumina Reduction Process
[O72] 16:20	*Viktoria Prostakova, Jeff Chen, Eugene Jak, Sergei A. Decterov* Development of a thermodynamic database for Ni-containing oxide systems for simulation of Ni extraction from laterite ores
16:40	**Coffee-break**
	Chairs Dr. Ursula R. Kattner Dr. Caroline Toffolon-Masclet
[O73] 17:00	*Herbert Ipser, Ratikant Mishra* The Ternary Ni-Sb-Sn System: Phase Diagram and Thermochemistry
[O74] 17:30	*Nils Warnken, Roger C Reed* A design driven Superalloy development approach
[O75] 17:50	*Alan J. Ardell* Interfacial Free Energies from Data on Coarsening Plus Assessments of Gibbs Free Energies of Mixing in Ni-Base γ/γ' Alloys
[O76] 18:10	*Dan Cai, Lijun Zhang, Yong Du* Phase-field simulation of grain growth in anisotropic systems
[O77] 18:30	*Jennifer M. Ullbrand, Bo Jansson, Ferenc Tasnádi, Lars Hultman, Magnus Odén* The effect of elastic anisotropy on the spinodal decomposition in (Ti,Al)N - a phase field study
[O78] 18:50	*Denis Shishin, Christopher Bale, Eugene Jak, Sergei A. Decterov* Thermodynamic database for copper smelting and converting
19:10	**Dinner**
20:30 22:30	**Poster Session**

Friday (Morning), May 27
Experiments and databases

	Chairs Prof. Zi-Kui Liu Prof. Bo Sundman
[O79] 08:30	*Rainer Schmid-Fetzer, Joachim Groebner, Artem Kozlov, Milan Hampl* Progress in magnesium alloy database development
[O80] 09:00	*Mamoun Medraj, Mohammad Mezbahul-Islam, Elhachmi Essadiqi* The Mg-Cu-Ni-Y quaternary system: thermodynamic modeling coupled with key experiments
[O81] 09:20	*M Jiang, HX Li, YP Ren, SM Hao* Experimental study on the long period ordered (LPO) phase in magnesium alloys
[O82] 09:40	*Ales Kroupa, Alan Dinsdale, Andrew Watson, Jan Vrestal, Adela Zemanova, Pavel Broz* The COST MP0602 Thermodynamic Database for High-Temperature Lead-free Solders
[O83] 10:00	*Leszek Zabdyr, Grzegorz Garzel* EMF Measurements in the Liquid Ag-Bi-Cu-Sn Lead-free Solder Alloys.
10:20	**Coffee-break**
	Chairs Dr. Suzana G. Fries Prof. Tomás Gómez-Acebo
[O84] 10:45	*Ursula R. Kattner, Bo Sundman, Mauro Palumbo, Suzana G Fries* Open Calphad - software and databases
[O85] 11:15	*Bengt Hallstedt* Thermodynamic evaluation of the Ti-Al-C system
[O86] 11:35	*Zi-Kui Liu, Zhi-Gang Mei, Vidvuds Ozolins* Lattice stability by ab initio molecular dynamic simulations
[O87] 11:55	*M Hindler and A. Mikula* Thermodynamic Properties of the Au-Sb-Sn and Au-Sb system
[O88] 12:15	*D. Kobertz, M. Müller* Experimental Studies and Re-assessment of the Quasi-binary Systems containing the Sulfates of Sodium, Potassium, and Calcium by Differential Thermal Analysis and X-Ray Diffraction
12:35	**Closing session**