# Conference Program

# Monday, June 1

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| 8:40 | | | **OPENING** | |
| | | | **Chair:** | **G. Cacciamani** |

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| | | | **SESSION 1:** | **Modeling 1** |
| | | | **Chairs:** | **Zi-Kui Liu, Malin Selleby** |
| 8:55 | O-01 | John | Agren | CALPHAD – Future Challenges |
| 9:10 | O-02 | In-Ho | Jung | Thermodynamics of Nitrogen in Molten Steel and Ferro-alloys |
| 9:25 | O-03 | Jean-Marc | Joubert | How much can be trusted a thermodynamic assessment done without any thermodynamic data? |
| 9:40 | O-04 | Blazej | Grabowski | Partitioning of Cr and Si between cementite particles and the ferrite matrix: An ab initio thermodynamics approach |
| 9:55 | O-05 | Rainer | Schmid-Fetzer | Inherently consistent temperature function for interaction parameters demonstrated for the Mg-Si assessment |
| 10:10 | | | | **Coffee-break** |

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| | | | **SESSION 2:** | **Ab initio 1** |
| | | | **Chairs:** | **Tetsuo Mohri, Emily Moore** |
| 10:30 | O-06 | Juan M. | Sanchez | Convergence Analysis of the Cluster Expansion |
| 10:45 | O-07 | Silvana | Tumminello | Using the Al-Ni binary system to explore the potentialities of first-principles quantities |
| 11:00 | O-08 | Marcel | Sluiter | Cluster expansions for configuration dependent kinetics in substitutional alloys |
| 11:15 | O-09 | Atsuto | Seko | Efficient determination of alloy ground-state structures |
| 11:30 | O-10 | Theresa | Davey | Fully anharmonic first principles data in the assessment of the B-C-Hf-Zr system |
| 11:45 | O-11 | B.-J. | Lee | An interatomic potential for ionic+covalent+metallic materials based on the modified embedded-atom method |
| 12:00 | | | | **Lunch** |

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| | | | **SESSION 3:** | **CALPHAD Assessments 1** |
| | | | **Chairs:** | **Ursula Kattner, Bo Sundman** |
| 14:00 | O-12 | Peter Franz | Rogl | The System Ti-Ni-Sn: Constitution and Thermodynamic Modelling |
| 14:15 | O-13 | Xuan | Liu | Experimental study and thermodynamic modeling of the Al-Co-Cr-Ni system |
| 14:30 | O-14 | Natacha | Bourgeois | High pressure modelling of the Ni-H system using first principle calculations |
| 14:45 | O-15 | Albina | Akhmetova | Thermodynamic modeling in Ag-Cu-Ge system |
| 15:00 | O-16 | Jana | Pavlu | Ab initio based thermodynamic modeling below room temperature: Hf-V system |
| 15:15 | O-17 | Luiz | Eleno | Thermodynamic modelling of the 1073K isotherm of the Nb–Ni–Si phase diagram using ab initio calculations |
| 15:30 | | | | **Coffee-break** |

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| | | | **SESSION 4:** | **Applications 1 (nano-materials and nuclear materials)** |
| | | | **Chairs:** | **Fernando Rizzo, Nathalie Dupin** |
| 16:00 | O-18 | Hyuck Mo | Lee | Anti-oxidation Property of Cu-Ag Core-Shell Nanoparticles Fabricated Using the Nano-Phase Diagram |
| 16:15 | O-19 | Nils | Warnken | Modelling of Phase Separation in Bi-metalic Nano Particles using the Cahn Hilliard Equation |
| 16:30 | O-20 | Masoomeh | Ghasemi | The phase diagram of the In-Sb nanoalloys |
| 16:45 | O-21 | Ales | Kroupa | Modelling of phase diagrams of nanoalloys with complex metallic phases: application to Ni-Sb-Sn system |
| 17:00 | O-22 | Patrice | Turchi | Ab initio Studies and Thermodynamic Assessment of Rare Earth-based Alloys |
| 17:15 | O-23 | Emily | Moore | Up to date assessment of thermodynamic data for nuclear materials |
| 17:30 | O-24 | Aurelien | Perron | CALPHAD assessments and inter-relationships between binary phase diagrams involving Al, Am, Ga, Pu, and U |
| 19:00 | | | | **Dinner** |
| 21:00 | | | | **POSTERS & DRINK SESSION 1**<br>Posters P1-P40 |

# Tuesday, June 2

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| | | | **SESSION 5:** | **Applications 2 (Geochemistry & Miscellaneous)** |
| | | | **Chairs:** | **Andre Schneider, Peter Miodownik** |
| 8:40 | O-25 | Surendra | Saxena | Thermodynamics of the binary Fe-S and Earth's core |
| 8:55 | O-26 | Donato | Belmonte | Performance of Hybrid Density Functionals in predicting thermodynamic properties of minerals at high pressure and high temperature |
| 9:10 | O-27 | Zhen | Nie | The prediction of mineral solubilities in natural waters: The Li-Na-SO 4 -CO 3 -H 2 O system at 298K |
| 9:25 | O-28 | Sergei | Decterov | Thermodynamic Modeling of Aluminosilicate Solid Solutions |
| 9:40 | O-29 | Andre | Costa e Silva | Failure of steel bolts in sub-sea application: a DICTRA investigation on microstructural banding and its the relevance to the failure |
| 9:55 | O-30 | James | Saal | Integrated Computational Materials Engineering of HighPerformance Co Alloys |
| 10:10 | | | | **Coffee-break** |
| | | | **SESSION 6:** | **Experiments 1** |
| | | | **Chairs:** | **Ikuo Ohnuma, Ales Kroupa** |
| 10:30 | O-31 | Yong | Du | Applications of TEM and 3DAP to measurement of phase equilibria: case studies for the Al-Fe-Ni-Si and Al-Mg-Si-Cu systems |
| 10:45 | O-32 | Mikael | Perrut | Coupling EDS mapping and diffusion multiples: towards a quick exploration of ternary phase diagrams |
| 11:00 | O-33 | Changjun | Wu | Linear and anisotropic growth of periodically layered structure in the Co2Si/Zn solid-liquid diffusion couples |
| 11:15 | O-34 | Dmitry | Sergeev | Thermodynamics of the Reciprocal System NaCl-KCl-NaNO3-KNO3 |
| 11:30 | O-35 | Hang | Wang | Growth of vaporisation induced recrystallised grains in Ni-base superalloys: experiments and thermodynamic calculations |
| 11:45 | O-36 | Ikuo | Ohnuma | Experimental Investigation of Miscibility Gap between Antiferromagnetic and Paramagnetic Phases in the NiMn-NiZn Pseudo-Binary System |
| 12:00 | | | | **Lunch** |
| | | | **SESSION 7:** | **Modeling 2** |
| | | | **Chairs:** | **Andre Costa e Silva, Bengt Hallstedt** |
| 14:00 | O-37 | Kiyohito | Ishida | Schaeffler-Type Phase Diagram of Ti-Based Alloys |
| 14:15 | O-38 | Jan | Vrestal | Combined quantum-mechanical and Calphad approach to description of heat capacity below room temperature |
| 14:30 | O-39 | Sedigheh | Bigdeli | Towards third generation Calphad databases: coupling between First Principles and Calphad calculations for case studies of Mn and Fe-Mn |
| 14:45 | O-40 | Hai-Lin | Chen | Modeling of ordered D03 with the 4SL partitioning model |
| 15:00 | O-41 | Florian | Tang | Modeling of the κ phase using a 4 sublattice model in the Al-FeMn-C system. |
| 15:15 | O-42 | Alan | Dinsdale | A new generation of data for the elements: Critical assessment of data for Zn and Cd |
| 15:30 | | | | **Coffee-break** |
| | | | **SESSION 8:** | **Ab initio 2** |
| | | | **Chairs:** | **Patrice Turchi, Jan Vrestal** |
| 16:00 | O-43 | Tetsuo | Mohri | Multi-scale Simulation of Order-Disorder Transformation in a binary alloy by Cluster Variation and Phase Field Methods |
| 16:15 | O-44 | Hiroshi | Ohtani | Calculation of the magnetic properties of anti-perovskite alloys |
| 16:30 | O-45 | Ali | Zendegani | First-principles study of thermodynamic properties of the Q phase in Al-Cu-Mg-Si |
| 16:45 | O-46 | Weiwei | Xu | Mechanical, thermodynamic properties and effects of alloying elements for Co-base γ¢ precipitates: A first principles study |
| 17:00 | O-47 | Jinghua | Xin | Site preference and diffusion of hydrogen during hydrogenation of Mg: A first–principles study |
| 17:15 | O-48 | Cathrine | Colinet | Enthalpies of formation of transition metal diborides. A first principles study |
| 17:30 | O-49 | Benjamin | Burton | First-principles phase diagram calculations for the Van der Waals dichalcogenide systems: MoS2-MoSe2, MoSe2-MoTe2, MoS2-MoTe2, and NbSe2-WSe2 |
| 19:00 | | | | **Dinner** |
| 21:00 | | | | **POSTERS & DRINK SESSION 2**<br>Posters P41-P80 |

# Wednesday, June 3

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| | | | **SESSION 9:** | **Thermodynamic databases 1** |
| | | | **Chairs:** | **Yong Du, Rainer Schmid-Fetzer** |
| 8:40 | O-50 | Ursula | Kattner | Capture Tools for Phase-based Data |
| 8:55 | O-51 | Richard | Otis | ESPEI: Open-source data infrastructure for Materials Genome |
| 9:10 | O-52 | Cassie | Marker | Thermodynamic database for Ti implant materials: With a focus on thermodynamic modeling of Ti-Ta-X systems |
| 9:25 | O-53 | Xiao-Gang | Lu | CALPHAD modelling of thermodynamic, diffusional and thermophysical properties for the Ni-Co-base alloys |
| 9:40 | O-54 | J.-Claude | Tedenac | Multicomponent Manganese silicides in a general CALPHAD approach |
| 9:55 | O-55 | Bengt | Hallstedt | Thermodynamic database for high-manganese steels |
| 10:10 | | | | **Coffee-break** |
| | | | **SESSION 10:** | **Experiments 2** |
| | | | **Chairs:** | **Zhenmin Du, Wladislaw Gasior** |
| 10:30 | O-56 | P M | Aiswarya | Thermochemical Studies on Pb-Mo-O System |
| 10:45 | O-57 | Yuwen | Cui | Screening of Microstructure and Property of Ti Alloys by Conceptual Diffusion Multiple Technique |
| 11:00 | O-58 | Andrea | Gil Santos | Experimental Investigation for the Thermodynamic Modeling of the Mg rich Corner in the Mg-Si-Sr System |
| 11:15 | O-59 | Shuhong | Liu | Experimental investigation and thermodynamic description of the Mg-RE-Zr systems |
| 11:30 | O-60 | Svetlana | Sinyova | Experimental approach to the phase diagrams construction is basis for the thermodynamic modelling |
| 12:00 | | | | **Lunch** |
| 14:00 | | | | **Social Tour** |
| 20:00 | | | | **Banquet** |

# Thursday, June 4

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| | | | **SESSION 11:** | **Thermodynamics & Software** |
| | | | **Chairs:** | **John Morral, Hiroshi Ohtani** |
| 8:40 | O-61 | Zi-Kui | Liu | Thermal expansion anomaly in ice and water |
| 8:55 | O-62 | Aimen | Gheribi | Prediction of the thermal conductivity of ionic materials by a new self consistent thermodynamics method. |
| 9:10 | O-63 | Konstantin | Starodub | Structure-based modelling of thermodynamic and physicochemical properties |
| 9:25 | O-64 | Peter | Miodownik | Encounters with Entropy |
| 9:40 | O-65 | Bo | Sundman | Some experiences and ideas for the development of a new assessment software |
| 9:55 | O-66 | Fan | Zhang | Application of the CALPHAD Method to Integrated Computational Materials Engineering |
| 10:10 | | | | **Coffee-break** |
| | | | **SESSION 12:** | **Diffusion & Surfaces** |
| | | | **Chairs:** | **Jhon Agren, In-Ho Jung** |
| 10:30 | O-67 | John | Morral | Multicomponent diffusivity validation with one diffusion couple |
| 10:45 | O-68 | Joonho | Lee | Wetting and Brazing of 304L Stainless Steel by Ag-Cu Eutectic Alloy under Ar Gas Atmosphere |
| 11:00 | O-69 | Rong | Wang | Eutectic solidification in Al-Ag-Cu alloys: DICTRA and phase-field simulation |
| 11:15 | O-70 | Jing-jing | Liu | Isothermal Wollastonite crystallization in CaO–Al2O3–SiO2 melts: a combination of phase field simulations with in-situ experiments |
| 11:30 | O-71 | Masanori | Kajihara | Isothermal Reactive Diffusion between Solid and Liquid Metals |
| 11:45 | O-72 | George | Kaptay | On the partial surface tension of components of a solution |
| 12:00 | | | | **Lunch** |
| | | | **SESSION 13:** | **Applications 3 (Miscellaneous)** |
| | | | **Chairs:** | **Kiyohito Ishida, Alan Dinsdale** |
| 14:00 | O-73 | Tim | Anderson | Phase Equilibria of the Ag-Cu-Ga-In System and Implications for Synthesis of Ag x Cu 1-x Ga y In 1-y Se 2 PV Absorber Layers |
| 14:15 | O-74 | Damian | Cupid | Thermochemistry of New Anode Materials for Li-Ion Batteries |
| 14:30 | O-75 | Hans | Flandorfer | Intermetallic Li-systems: Experimental challenges and results |
| 14:45 | O-76 | Maren | Lepple | Thermochemistry of Copper Oxides and Lithium Copper Oxides for Use as Electrode Materials in Lithium Ion Batteries |
| 15:00 | O-77 | Kaj | Thomsen | Modeling the solubility of ammonium and magnesium phosphates in multi-component solutions with the Extended UNIQUAC model |
| 15:15 | O-78 | Dhanesh | Chandra | Continuous Solid-State Phase Transitions in Energy Storage Materials with Orientational Disorder – Computational and Experimental Approach |
| 15:30 | | | | **Coffee-break** |
| | | | **SESSION 14:** | **CALPHAD Assessments 2** |
| | | | **Chairs:** | **George Kaptay, Hyuk Mo Lee** |
| 16:00 | O-79 | Olga | Fabrichnaya | Thermodynamic descriptions for the Zr-Mn-Mg-O system based on experimental data |
| 16:15 | O-80 | Bonnie | Lindahl | Thermodynamic re-assessment of the Al-V system towards an assessment of the Al-Ti-V system |
| 16:30 | O-81 | Soumya | Sridar | Thermodynamic modeling of Ti-Zr-N coupled with first principle calculations |
| 16:45 | O-82 | Hongqun | Dong | Experimental study of the Au-20wt.%Sn\|Pt interconnection and thermodynamic reassessment of the Au-Pt-Sn ternary system |
| 17:00 | O-83 | Song-Mao | Liang | Challenges in the thermodynamic assessment of the Al-Cu-Zn system |
| 17:15 | O-84 | Lars K. | Jakobsson | Key experiments and a critical thermodynamic evaluation and optimization of the iron saturated FeO-B2O3-Nd2O3 system |
| 17:30 | O-85 | Alexandra | Khvan | Thermodynamic assessments and experimental investigations of the Fe-Ce-C and Fe-La-C systems |
| 19:00 | | | | **Dinner** |
| 21:00 | | | | **POSTERS & DRINK SESSION 3**<br>Posters P81-P120 |

# Friday, June 5

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| | | | **SESSION 15:** | **Experiments 2** |
| | | | **Chairs:** | **Peter Rogl, Olga Fabrichnaya** |
| 8:40 | O-86 | Sinn-Wen | Chen | Phase diagrams of the Co-Sb-X thermoelectric materials systems; Phase diagram determinations of the N-type Bi-Se-Te-x alloys |
| 8:55 | O-87 | Mikhail | Sheindlin | Study of High-Temperature Phase Diagram of Zr-C System in the Domain of Solid Solution by Laser-Pulse Melting |
| 9:10 | O-88 | Susan V. | Meschel | The thermochemistry of some binary lead and lanthanide metal compounds by high temperature direct synthesis calorimetry. |
| 9:25 | O-89 | Mario | Kriegel | Thermodynamic investigations in the binary Al-Mo and ternary Al-Mo-Ti System |
| 9:40 | O-90 | Dietmar | Kobertz | Thermodynamic Vaporization Studies on Mn-doped Lead Titanate and Sodium Niobate |
| 9:55 | O-91 | Aurélie | Jacob | Investigation in the Cr-Fe-Nb phase diagram |
| 10:10 | | | | **Coffee-break** |
| | | | **SESSION 16:** | **Databases 2** |
| | | | **Chairs:** | **Byeong-Joo Lee, Bo Sundman** |
| 10:30 | O-92 | Elena | Yazhenskikh | Development of a new thermodynamic database for slag relevant oxide systems containing SO3 |
| 10:45 | O-93 | Jun | Zhu | Thermodynamic Database for High Temperature Co-Based Superalloys |
| 11:00 | O-94 | Eugenio R. | Pinatel | Thermodynamic database for borohydrides: present knowledge and future challenges |
| 11:15 | O-95 | Lijun | Zhang | A quantitative and efficient phase-field model with finite interface dissipation |
| 11:30 | | | **CONCLUSION** | |
| | | | **Chair:** | **G. Cacciamani** |
| 12:00 | | | | **Lunch** |
| 14:00 | | | | **Visit of Ansaldo Energia** |