

**PROGRAM AND ABSTRACTS**



**CALPHAD**  
**XXXVI**

THE PENNSYLVANIA STATE UNIVERSITY  
STATE COLLEGE, PENNSYLVANIA  
MAY 6-11, 2007





Welcome to

# **CALPHAD XXXVI**

**The Pennsylvania State University**

## **Organizing Committee**

Professor Zi-Kui Liu (The Pennsylvania State University)

Dr. Steve Hansen (APL Engineered Materials, Inc.)

Dr. Joanne Murray (ALCOA)

Dr. Philip Spencer (The Spencer Group)

# Sponsors

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Calphad, Inc.

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Materials Research Institute, The Pennsylvania State University

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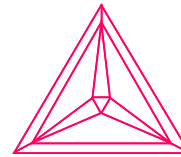
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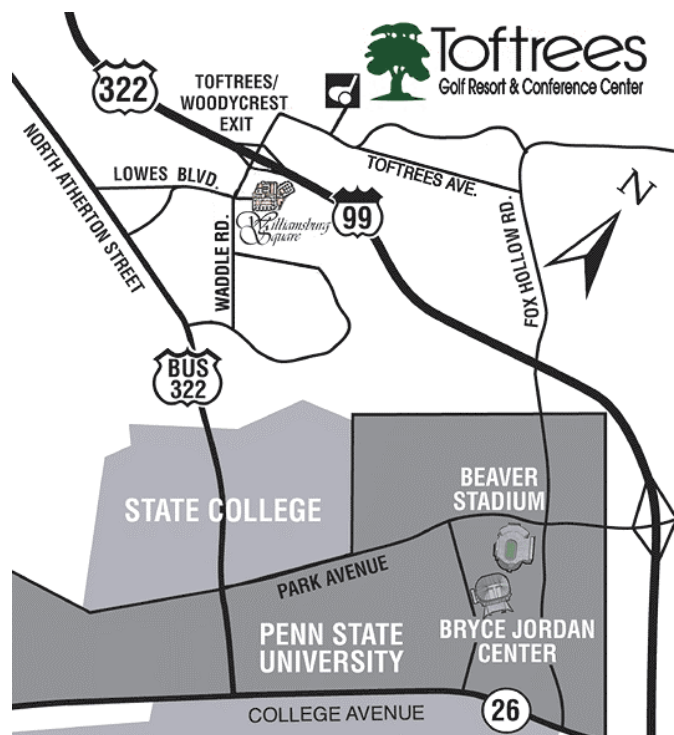
## General Information

### **Toftrees Contact Information**

CALPHAD XXXVI will be held at the Toftrees Golf Resort and Conference Center in State College, Pennsylvania. Participants can enjoy the conference facilities: an 18 hole golf course, driving range, lighted tennis courts, fitness center, spa, restaurant and business center.

The Conference contact information is:

Toftrees Golf Resort & Conference Center  
One Country Club Lane  
State College, Pennsylvania 16803  
Toll Free: (800) 252-3551  
Local: (814) 234-8000  
Fax: (814) 238-4404  
Email: [info@toftrees.com](mailto:info@toftrees.com)

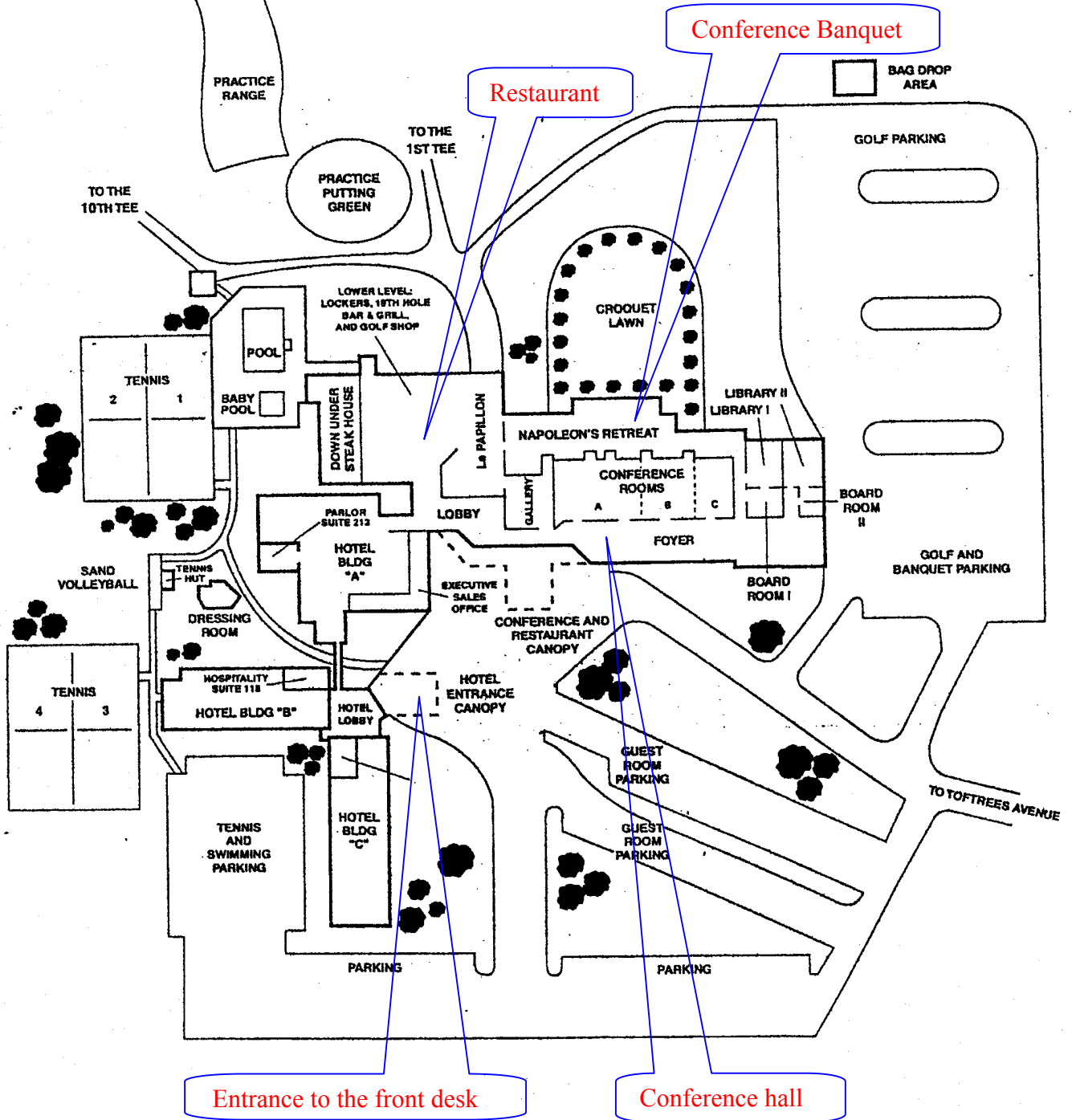


### **Registration and Information**

The registration desk will be open on:

Sunday, May 6	3:00 PM – 6:30 PM, Front Desk
Monday, May 7	8:00 AM– 5:00 PM, Next to Conference Hall

# Map of Toftrees



## ***Poster Instructions***

The posters will be on display from Sunday evening until Friday morning in the conference room and the foyer. Poster size should be 36" × 48" (90 × 120 cm) in either portrait or landscape format. Poster boards and Velcro will be provided. In addition to the continuous display of the posters, two dedicated poster sessions will be held in the Monday and Tuesday evenings from 20:00 to 21:30 (8:00 – 9:30 pm). Posters should be mounted on the poster boards no later than Monday before 16:45. Poster should be removed before Friday noon.

## ***Transportation***

Transportation to and from the State College Airport is provided by a shuttle operated by Toftrees. Please contact the hotel for your arrival and departure shuttle services.

## ***Taxi Services***

Taxi By Handy Delibery	(814) 353-6001
Nittany Express Inc	(814) 867 4647
Aa Transit Inc.	(814) 231-8294

## ***Accompanying Persons Program***

- ***Monday, May 7:*** Excursion to Penn's Cave and Wild Life Park. This trip will include a tour of a water cavern by boat.
- ***Tuesday, May 8:*** Excursion to a local winery and shopping in nearby Altoona, Pennsylvania.
- ***Thursday, May 10:*** Excursion to Victorian Bellefonte – This will include a tour of sites in nearby Bellefonte, Pennsylvania.

## ***Electricity***

U.S. voltage operates at 110 volts.

## ***Currency Exchange***

Citizens Bank, 122 West College Avenue, State College, PA 16801

Hours: Monday-Thursday: 9AM-5PM, Friday: 9AM-6PM, Saturday: 9AM-12PM, Sun: closed

Phone: 814-234-6311

## ***Internet Service***

The hotel lobby has wireless access as well as the ballroom. In the guestrooms you would need a land line.

# Conference Program

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***Sunday, 6 May 2007***

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15:00 – 18:30      Registration

19:30              Welcome Reception at Toftrees Restaurant (see map)

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**Monday, 7 May 2007**

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**7:00 – 8:15**            *Breakfast*

**8:20**            **Opening Remarks**            **Zi-Kui Liu**

08:30 – 10:10            **Session: Thermodynamic Modeling (I)**  
**Chairs: Nathalie Dupin, Philip Spencer**

08:30 Alan Dinsdale: The Problem with Vacancies - Data for Nothing!

08:55 Arthur Pelton: Modeling Short-Range Ordering

09:20 Tooru Matsumiya: A Proposal of Evaluation Method of energy Parameter Values in Cell Model for Refining Slag

09:45 Xiaogang Lu: A Unified Description of Thermo-Physical Properties

**10:10 – 10:40**            *Coffee Break*

10:40 – 12:20            **Session: Thermodynamic Modeling (II)**  
**Chairs: Karin Frisk, Marko Hamalainen**

10:40 P.E.J. Rivera Diaz del Castillo: Level Set Method for Particle Growth and Dissolution in Multicomponent Non-ideal Alloys

11:05 Tatsuya Tokunaga: Thermodynamic Analysis of the Fe-Zr-B Ternary System

11:30 Eli Brosh: Equation of State for CALPHAD Modelling, Application to Elements and Alloys

11:55 Shigeto Nishitani: Driving Force in Metastable Solvent Epitaxy

**12:20 – 13:30**            *Lunch*

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**Monday, 7 May 2007**

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13:40 – 15:25      **Session: Energy Materials**  
**Chairs: Steve Hansen, Alexandra Kusoffsky**

13:40 Ursula R. Kattner: Challenges in the Development of a Thermodynamic Database for Metal-Hydrogen Systems

14:05 Mauro Palumbo: Thermodynamic and *ab initio* Study of the Al, Mg, Na, B-based Systems for Hydrogen Storage

14:30 Ming Chen: Reaction Thermodynamics at LSM-YSZ Interface in SOFCs

14:55 Dietmar Kobertz: Phase Diagram Determination of the Quasi-binary System TlI-DyI<sub>3</sub> by Differential Thermal Analysis

**15:20 – 15:50      *Coffee Break***

15:50 – 17:55      **Session: *ab initio* Calculations**  
**Chairs: Mojmir Sob, Hui Zhang**

15:50 Jan Vrestal: Lattice Stabilities of Laves Phases in Chromium Alloys

16:15 Claudio Geraldo Schon: *ab initio* Calculation of the Ti-Fe (Titanium-Iron) Phase Diagram and the Stability of the B<sub>2</sub>-TiFe Compound

16:40 Raymundo Arroyave: Application of *ab initio* Finite Temperature Thermodynamics to CALPHAD Modeling

17:05 Mark Asta: *ab initio* Molecular Dynamics Simulations of Molten Superalloys

17:30 Maoyou Chu: *ab initio* Study of the Phase Transition Spinel of Li<sub>x</sub>Mn<sub>2</sub>O<sub>4</sub>

**18:30                      *Dinner***

**20:00–21:30              **Poster Session with wine and cheeses****

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**Tuesday, 8 May 2007**

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**7:00 – 8:15**            *Breakfast*

08:30 – 10:10           **Session: Modeling of Materials Properties**  
**Chairs: Bengt Hallstedt, Rainer Süss**

08:30 Nicholas Grundy: Modeling the Viscosity of Aluminosilicate Melts

08:55 Risto Pajarre: Modelling of Surface and Interfacial Phenomena Using a Multi-Phase Free Energy Minimization Model

09:20 Zbigniew Moser: Wettability Studies of Sn-Ag-Cu-In Liquid Solders and Interaction with Cu Substrate

09:45 John Morral: Teaching Phase Diagram Topology to Undergraduates

**10:10 – 10:40**           *Coffee Break*

10:40 – 12:20           **Session: Diffusion and Phase-Field Simulations**  
**Chairs: Toru Miyazaki, Christian Robelin**

10:40 Long-Qing Chen: Predicting Precipitate Microstructure Evolution Starting from First-Principles

11:05 Testuo Mohri: Phase Field Calculations Combined with Cluster Variation Method

11:30 Nele Moelans: Phase Field Simulations of the Pinning Effect of Second-Phase Particles on Grain Boundaries: Effect of Particle Shape, Stability and Interfacial Properties

11:55 Manjeera Mantina: Calculating Diffusion Coefficients in Pure Metals and Dilute Binary Alloys Exclusively via a First-Principles Approach

**12:20 – 13:30**           *Lunch*

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**Tuesday, 8 May 2007**

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13:40 – 15:20      **Session: Ni-base Superalloys**  
**Chairs: Suzana Fries, Kiyohito Ishida**

13:40 Carelyn Campbell: Successes and Challenges in the Development of a Diffusion Mobility Database for Ni-base Superalloys

14:05 Tomás Gómez-Acebo: Experimental and Computational Study of Precipitates Growth in Inconel 718 and Allvac 718Plus Superalloys

14:30 Evan Copland: Solidification Behaviour of  $\gamma'$ -Ni<sub>3</sub>Al Containing Alloys in the Ni-Al-O System

14:55 Rada Novakovic: Surface and Transport Properties of Al-Cr-Ni Liquid Alloys

**15:20 – 15:50      *Coffee Break***

15:50 – 17:55      **Session: Modeling of Al, Ti, Steel, and Electronic Materials**  
**Chairs: Mamoun Medraj, Joanne Murray**

15:50 Bo Sundman: Modelling the Al-Ti System

16:15 David Sedmidubsky: Thermodynamic Aspects of GaN-Based Dilute Magnetic Semiconductors

16:40 Jean-Claude Tedenac: Experimental Investigation and Thermodynamic Modelling of the Ti-Si-Sn System

17:05 Jozefien De Keyzer: Thermodynamic modeling of the Fe-Ni-Ti system using a 4-sublattice model

17:30 Yong Du: The Al-Ce-Mn-Ni quaternary system: thermodynamic modeling supported by key experiment

**18:30                      *Dinner***

**20:00–21:30              **Poster Session with wine and cheeses****

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**Wednesday, 9 May 2007**

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**7:00 – 8:00**    *Breakfast*

08:00            Depart from Hotel Lobby for one day tour of Gettysburg

11:00            Arrive Gettysburg

16:00            Leave Gettysburg

19:00            Arrive Toftrees

19:30            Social Gathering

20:00            Barbeque Dinner at the Napoleon's Retreats (see the Toftrees map)

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**Thursday, 10 May 2007**

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**7:00 – 8:15**            *Breakfast*

08:30 – 10:10           **Session: Modeling of Nano Materials**  
**Chairs: Gabriele Cacciamani, Caroline Toffolon-Masclet**

08:30 Byeong-Joo Lee: Thermodynamics of Nano Materials

08:55 Pierre Perrot: Thermodynamics of Metal-Semiconductor Systems in the Nanometer Range and its Application to the Mechanism of Semiconductor Nanowire Growth

09:20 Hyuck Mo Lee: Phase Stability of the Bimetallic Nanocluster: Genetic Algorithm, Basin-Hopping Monte Carlo and Molecular Dynamics Study

09:45 Toru Miyazaki: A Phase Diagram Based upon the Non-Extensive Entropy and Its Application to the Phase Decomposition Process

**10:10 – 10:40**            *Coffee Break*

10:40 – 12:20           **Session: Bulk Metallic Glass and Liquid**  
**Chairs: Michel Jacobs, Lina Kjellqvist**

10:40 Larry Kaufman: Calculation of Kinetic Factors Controlling the Stability and Pourbaix Diagrams of HPCRM Alloys

11:05 Joe Farmer: The Electrochemical Response of Passive Films on Families of Iron-Based Amorphous Metals with Various Levels of Chromium, Molybdenum, Tungsten and Yttrium

11:30 Kjetil Hildal: Thermal Stability of an Fe-based Bulk Metallic Glass: Thermodynamic Modelling and Experimental Verification

11:55 Jean-Philippe Harvey: Thermodynamic Modeling of Hydrogen Solubility in Aluminum Melts

**12:20 – 13:30**            *Lunch*

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**Thursday, 10 May 2007**

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13:40 – 15:25      **Session: Applications to Materials Discovery and Design**  
**Chairs: John Vitek, Jor-Shan Choi**

13:40 Ping Wu: Materials Discovery through Integrated Multidisciplinary and Multiscale Modeling

14:05 André Schneider: Effect of the titanium and nitrogen content on the formation of primary TiN precipitates during the solidification of microalloyed steels

14:30 Wei Xu: Design of Precipitation Hardened Maraging Steels through Alloy Combinatorial Approaches and Precipitate Distribution Optimisation

14:55 Hideaki Ikehata: Simulation of Carbide Growth by Carbide-dispersion Carburizing (CDC) Process

**15:20 – 15:50      *Coffee Break***

15:50 – 17:55      **Session: Applications to Materials Processing**  
**Chairs: André Schneider, Nele Moelans**

15:50 Rainer Schmid-Fetzer: Phase Formation in Monotectic Al-Cu-Sn Based Alloys

16:15 Roberto de Avillez: The Effect of Alloying Elements on the Kinetics of Carbon Enrichment of Retained Austenite in TRIP-like Steels

16:40 Muhammad A. Arafin: Coupling Kinetics with Multicomponent Thermodynamics to Model Isothermal Solidification during TLP Bonding of Nickel Superalloys and Stainless Steels

17:05 Andre Costa e Silva: The Thermodynamics of Calcium and Magnesium in Iron and its Implications on Secondary Steelmaking

17:30 Tim Anderson: Thermodynamic Database for the Cu-Ga-In-Se System

**18:30                      *Dinner***

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**Friday, 11 May 2007**

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**7:00 – 8:15**            *Breakfast*

08:45 – 10:25        **Session : Modeling of Oxides**  
**Chairs: Patrice Chartrand, Viktoria Reiter**

08:45 Gunnar Eriksson: From SOLGAS to FactSage - An Overview

09:10 Stephan Petersen: Process Simulation Applications with SimuSage

09:35 Erwin Povoden: Thermodynamic Assessment of the La-Cr-O and LaO<sub>3/2</sub>-MnOx-CrO<sub>3/2</sub> Systems

10:00 Samuel Hallstrom: Modelling and Simulation of Diffusion in Iron Chromium Oxides

**10:25 – 10:55**            *Coffee Break*

10:55 – 12:35        **Session : Applications to Oxide-related Systems**  
**Chairs: Yu Zhong, Zi-Kui Liu**

10:55 Franz Melcher: Investigations of Refractory/Slag Equilibria in Steel Ladles

11:20 Lakshmi Narasimhan: Mass Spectrometric Study of Vaporization Behavior Associated with Condensed Phase Transitions and Information on Phase Diagrams

11:45 CALPHAD XXXVII - Finland Presentation - Marko Härmäläinen

12:10 Closing Ceremony – Larry Kaufman

**12:35 – 14:00**            *Lunch*

## Oral Presentation Abstracts

- Alan Dinsdale: The Problem with Vacancies - Data for Nothing!
- Arthur Pelton: Modeling Short-Range Ordering
- Tooru Matsumiya: A Proposal of Evaluation Method of energy Parameter Values in Cell Model for Refining Slag
- Xiaogang Lu: A Unified Description of Thermo-Physical Properties
- P.E.J. Rivera Diaz del Castillo: Level Set Method for Particle Growth and Dissolution in Multicomponent Non-ideal Alloys
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- Jan Vrestal: Lattice Stabilities of Laves Phases in Chromium Alloys
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- Mark Asta: Ab-Initio Molecular Dynamics Simulations of Molten Superalloys
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- Nicholas Grundy: Modeling the Viscosity of Aluminosilicate Melts
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- John Morral: Teaching Phase Diagram Topology to Undergraduates
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Samuel Hallstrom: Modelling and Simulation of Diffusion in Iron Chromium Oxides  
Franz Melcher: Investigations of Refractory/Slag Equilibria in Steel Ladles  
Lakshmi Narasimhan: Mass Spectrometric Study of Vaporization Behavior Associated with Condensed Phase Transitions and Information on Phase Diagrams

## Poster Presentation Abstracts

- P.1. Taichi Abe: Thermodynamic Assessment of the Ir-based Systems
- P.2. Ondrej Benes: Thermodynamic Study of the LiF-NaF-RbF-CsF-LaF<sub>3</sub> System
- P.3. Pavel Broz: Theoretical and Experimental Study of the Ni-Al-Ti System
- P.4. Gabriele Cacciamani: Drawbacks and Difficulties in the Investigation of the Magnesium Alloys by High Temperature Calorimetry
- P.5. Gabriele Cacciamani: Experimental Investigation and Thermodynamic Modelling of the Au-In-Sn System
- P.6. Jor-Shan Choi: Radiation Effect of Neutron-Absorbing Amorphous Metal Ribbons and Coatings
- P.7. Roberto de Aveliz: The Effect of Alloying Elements on Carbon Constrained Equilibrium due to a Quench and Partition Process
- P.8. Suzana Fries: Refining the Thermodynamic Description of the Ti-Sn Binary System
- P.9. Karin Frisk: The Solubility of Carbonitrides in Steel
- P.10. Michael Gao: Effect of Applied Microwave Energy on the Phase Equilibria of C-Co-W System
- P.11. Wladyslaw Gasior: Calorimetric Studies of the Enthalpies of the Formation of Intermetallic Phases from Al-Fe-Ni-Ti System
- P.12. Nicholas Grundy: Assessment of B<sub>2</sub>O<sub>3</sub> Containing Systems
- P.13. Bengt Hallstedt: Thermodynamic Evaluation of the Al-Li-Mg System, Including Volume Data
- P.14. Tuomas Hirsi: Improving Inclusion Tracking in Steel Flow with Combined CFD and Thermodynamics
- P.15. Takayuki Honda: Thermodynamic modelling of the Ni<sub>3</sub>Fe phase in the Fe-Ni System
- P.16. Rongxiang Hu: Calorimetric Study of Al-Ni-Ti System
- P.17. Hideki Ishii: Concentration of Profile Simulation of Metastable Solvent Epitaxy
- P.18. Md. Mezbahul Islam: Thermodynamic Modeling of the Mg-Cu-Y System
- P.19. Toni Ivas: Experimental Phase Diagram and Thermodynamic Assessment of the Gd<sub>2</sub>O<sub>3</sub>-CoO System
- P.20. Michel Jacobs: Phase Behavior in the System Fe-Al
- P.21. Andreas Janz: Experimental Investigation and Thermodynamic Modeling of Relevant Subsystems of the Mg-Al-Ca-Sr System
- P.22. Min Jiang: An Estimation of the Thermodynamic Stability of  $\gamma'$  Co<sub>3</sub>(Al,W) in the Co-Al-W System
- P.23. Jean-Marc Joubert: Thermodynamic Assessments of the Palladium-Hydrogen, Palladium-Deuterium and Palladium-Tritium Systems
- P.24. Julien Jourdan: Thermodynamic Assessment of the Zr-Er Binary System
- P.25. Youn-Bae Kang: Thermodynamic Databases for Magnesium Alloy Design
- P.26. Youn-Bae Kang: Experiment and Thermodynamic Optimization of the MnO-SiO<sub>2</sub>-"TiO<sub>2</sub>"-"TiO<sub>2</sub>O<sub>3</sub>" System for Application to Steel Production

- P.27. Lina Kjellqvist: Thermodynamic Assessment of the Aluminum-Titanium-Oxygen System
- P.28. Pertti Koukkari: Constrained Gibbs Energy Models for Some Intricate Systems
- P.29. Alex Kroupa: The Experimental and Theoretical Study of the Pd-Sn-Zn System
- P.30. Alexandra Kusoffsky: On the N Solubility in WC
- P.31. Guillaume Lambotte: Thermodynamic Assessment of the Alumina-Sodium Oxide-Silica System Using the Modified Quasi-chemical Model
- P.32. Byeong-Moon Lee: Thermodynamic Study of Phase Equilibria in the Fe-B-N Ternary System
- P.33. Sung Hoon Lee: The thermodynamic and first-principles study of magnesium substituted lithium borohydride for hydrogen storage material
- P.34. Chunlei Liu: Thermodynamic Assessment and Experimental Investigation of the Cu-Sn-Ti System
- P.35. Dmitri V. Malakhov: A Particular Type of Post-optimization Artifacts and Approaches to their Elimination
- P.36. Annelies Malfliet: Investigation of the Controversial Fe<sub>3</sub>Nb<sub>3</sub>-Phase in the Fe-Cr-Nb System
- P.37. Kinichi Masuda-Jindo: First Principles Calculations of Thermodynamic Quantities and Phase Diagrams of High Temperature BCC Mo-Ta-W Alloys
- P.38. Nele Moelans: A Comparison between Continuum Field and Multi-phase Field Models for Grain Growth
- P.39. Nele Moelans: Determination of the Ga-In-Si phase Diagram for the Growth of Si Nanowires via a Vapour-Liquid-Solid Technique
- P.40. Joanne Murray: Precipitation Models and Phase Diagrams for Industrial Aluminum Alloys
- P.41. Atsushi Nishikawa: First Principles Calculations of Solute Atoms in bcc-Fe
- P.42. Jan Jerzy Norwicz: Consistency of Measurements Data
- P.43. Ikuo Ohnuma: Thermodynamic Database of High-strength Low-Density Steels
- P.44. Jonas Östby: Thermodynamic Modelling of the CoO-Cr<sub>2</sub>O<sub>3</sub> System
- P.45. Ximiao Pan: Simulations of Ni-Cr-Al Diffusion Couples Compared with Experimental Results
- P.46. Erwin Povoden: The Bi<sub>2</sub>O<sub>3</sub>-Sb<sub>2</sub>O<sub>3</sub>-ZnO Phase Diagram at 1115 oC in Air
- P.47. Johannes Preußner: Thermodynamic Calculations on the Cr-Ni-Pt System
- P.48. Viktoria Reiter: Thermochemical Characterisation of Fayalite Slags of the Non-ferrous Industry and Refractory/slag Equilibria
- P.49. Christian Robelin: A Viscosity Model for the Na<sup>+</sup>, Al<sup>3+</sup>, Ca<sup>2+</sup>/F<sup>-</sup>, O<sup>2-</sup> Electrolyte
- P.50. Malgorzata Rys: Study of the high Na<sub>2</sub>O Concentration Part of the Na<sub>2</sub>O-SiO<sub>2</sub> System by Differential Thermal Analysis
- P.51. Ji-Hoon Ryu: Surface Segregation in the Bimetallic Cluster: Effect of Relative Cohesive Energy, Surface Energy and Atomic Radius
- P.52. Inyoung Sa: A Thermodynamic Approach for the Size-Dependent Composition Variation of Si-Ge Nanowire
- P.53. James Saal: A Thermodynamic Assessment of the Boron-Carbon System with First-Principles

- P.54. Arkapol Saengdeejing: Effect of Carbon in MgB<sub>2</sub> Thin Films: Intrinsic or Extrinsic
- P.55. Akira Sakamoto: Kinetic Simulation of Metastable Solvent Epitaxy
- P.56. Claudio Geraldo Schon: A Generalized Thermodynamics Formulation of the Cluster Variation Method
- P.57. David Sedmidubsky: Thermodynamic Properties of Strontium Niobates and the Assessment of SrO-Nb<sub>2</sub>O<sub>5</sub> Phase Diagram
- P.58. An Serbruyns: Experimental Study of the Phase Equilibria in the Aluminum-Nickel-Titanium System by Means of the Diffusion Couple Technique
- P.59. Shunli Shang: First-principles Calculations of Phonon and Thermodynamic Properties in B-As System
- P.60. Guang Sheng: Coarsening kinetics with large difference in diffusional mobilities of two phases
- P.61. Dongwon Shin: Phase stability of hafnium oxide and zirconium oxide on silicon substrate
- P.62. Dongwon Shin: Thermodynamic properties of fcc solution phases from Special Quasirandom Structures
- P.63. Adarsh Shukla: Thermodynamic Optimization and Evaluation of Mg-Si-X (X=Zn, Ce, Y, Mn) Systems for Use in Automotive Industry
- P.64. Moimir Sob: Ab Initio Study of the bcc-fcc and bcc-hcp Phase Transformations in Magnetically Ordered Iron
- P.65. Bo Sundman: Computational Thermodynamics - The Calphad Method
- P.66. Rainer Süss: Ongoing Development of the Thermodynamic Database for Pt-based superalloys
- P.67. Ryohei Takeda: First Principles Calculations of SiC Vibrational Free Energy
- P.68. Sherali Tursunbadalov: Forecast of Common (Balanced) Crystallization of Salts in Systems Consisting of Sulfates, Carbonates, Bicarbonates and Fluorides of Sodium and Potassium
- P.69. Jan Vrestal: Thermodynamic Modeling in the Cu-In-Sn System
- P.70. Yi Wang: Ab initio Calculations of Thermodynamic Properties
- P.71. Tom Woodcock: Solidification in Undercooled Metallic Droplets: Recent Results from Terrestrial and Parabolic Flight Experiments
- P.72. Johan Zander: Modelling mechanical properties for non-hardenable aluminium alloys
- P.73. Adela Zemanova: Thermodynamic Reassessment of the Cu-Ni-Sn System
- P.74. Hui Zhang: Avoid the appearance of artificial inverted miscibility gaps in the Mg-Si system
- P.75. Lijun Zhang: Experimental Investigation and Thermodynamic Description of the Al-Fe-Ni System over the Entire Temperature and Composition Ranges
- P.76. Mohammad Aljarrah: Thermodynamic Modeling of the Magnesium-Aluminum-Calcium-Strontium System Using Quasi-chemical Model
- P.77. Yong Du: Microstructure and mechanical properties of CrN and (Cr, Al)N coatings
- P.78. Damian Cupid: Thermodynamic Calculations for the Design of High-Temperature Ti-Al-Nb Based Alloys
- P.79. Yongzhang Huang: Thermodynamic Properties and Phases Relations of Ni-Sb Alloys
- P.80. Mei Li: Thermodynamic Assessment of the Pt-Ti System

- P.81. Xinjun Liu: Thermodynamic Assessment of Phase Equilibria in the Sn-Ag-X (Au, Ni) System
- P.82. Xinjun Liu: Experimental Determination and Thermodynamic Calculation of the Phase Equilibria in the Co-Mo-X (X: Al, Fe, Ni and W) System
- P.83. Ya Liu: An atomistic study on the structure of FeZn<sub>13</sub> and site preference of ternary elements
- P.84. Jianyun Shen: Thermodynamic Optimization of the Quasi-binary CuGaSe<sub>2</sub>-CuInSe<sub>2</sub>

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