PROGRAM BOOKLET

Computer Coupling of Phase Diagrams and Thermochemistry

CALPHAD XLIII

June 1\textsuperscript{st} to June 6\textsuperscript{th}, 2014

Changsha, Hunan, CHINA
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ORGANIZED BY

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State Key Laboratory of Powder Metallurgy

International Exchange and Cooperation, Central South University

China

June 1st to June 6th, 2014
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Acknowledgments:

Thanks are due to Yuehui He, Wensheng Liu, Xiang Xiong, Yong Liu, Duxin Li, Min Song, Zuming Liu, Maozhong Yi, Qizhong Huang, Kanghua Chen, Jianming Ruan, Yongjun Xiong, Zhijian Liu, Muyue Zhao (State Key Lab of Powder Metallurgy); Shuquan Liang, Danqing Yi (School of Materials Science and Engineering); Zhongyang Tang, Qihou Li, Houping Wu, Yan Yang, Zhiming Yu, Jufang Huang, Hongying Xie (Central South University Authority) for their suggestions and support during the organization of CALPHAD XLIII.

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SOCIAL PROGRAM (for accompanying people)

Sunday, June 1\textsuperscript{st}
- 19:30 Welcome cocktail at Empark Grand Hotel

Monday, June 2\textsuperscript{nd}
- 08:30 Bus tour of Changsha City, and visit famous Xiang Embroidery Exhibition - Hunan Xiang Embroidery Institute
- 12:00 Lunch at Fire Palace -- Taste famous local specialties
- 14:00 Visit Orange Island
- 18:00 Dinner at Empark Grand Hotel

Tuesday, June 3\textsuperscript{rd}
- 08:30 Go to Yueyang City, and visit Yuyeyang Pavilion
- 10:30 Visit Sanzui Pavilion, Xianmei Pavilion, Xiaqiao Tomb, Dongting Lake, etc.
- 12:00 Lunch in Junshan Island -- A beautiful place inside Dongting Lake
- 14:00 Visit Two concubines (E’huang & Nvying) tomb, Bamboo Forest, etc.
- 16:00 Returning to Changsha
- 18:20 Dinner at Empark Grand Hotel

Wednesday, June 4\textsuperscript{th}
- 09:00 Go to pedestrian zone for sightseeing and shopping at city center
- 12:40 Lunch at Empark Grand Hotel
- 13:30 Conference Excursion
- 18:00 Conference Dinner at Empark Grand Hotel

Thursday, June 5\textsuperscript{th}
- 08:30 Go to Shaoshan, and visit Chairman Mao’s hometown and Statue
- 12:00 Lunch in Shaoshan
- 13:00 Visit Dropping Water Cave
- 14:30 Take bus to Huaming Mansion --- Shaoqi Liu’s hometown
- 16:00 Returning to Changsha
- 18:10 Dinner at Empark Grand Hotel

Friday, June 6\textsuperscript{th}
- 13:00 Lunch at Empark Grand Hotel
CALPHAD XLIII, Changsha, Hunan, China, June 1st to June 6th, 2014

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<td>S8: Microstructure Characterization &amp; Simulation (I)</td>
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<td>Welcome Cocktail</td>
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<td>Software Demonstration Session</td>
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Venue

Empark Grand Hotel (世纪金源大饭店)

No. 199 Jintai Road, Kaifu District, Changsha 410008, P.R. China
(中国湖南长沙市开福区金泰路199号)
Tel.: +86 731 8595 8888
Fax.: +86 731 8598 9999
http://www.empark.com.cn/

Conference Excursion

On Wednesday, June 4th, the Conference will be interrupted for a half-day excursion that will include a visit of Kaifu Temple (开福寺), Yuelu Academy (岳麓书院) and Aiwan Pavilion (爱晚亭), as well as a sightseeing along Xiangjiang River.

Kaifu Temple --- Located in the north suburbs of ancient Changsha city (now almost in the center of the city), first built in the Five Dynasties Ten Countries period (909-979) of thousand years of history. The Temple was and is always the most important palace for religious activities and the best place to pray for peace and happiness for human beings.

开福寺：坐落在古长沙城北，为禅宗临济宗杨岐派著名寺院，始建于五代时期，距今已有一千多年历史。自建寺以来，虽几经损毁，开福寺的香火一直绵延不绝，佛事兴盛。特别是成为比丘尼丛林以来，在方丈能净法师的主持下，弘扬正法，广利众生，法门昌盛，声名远播，是中国佛教重点开放寺院之一。如今的开福寺已经在长沙城内，正在以其千年古刹之丰厚底蕴，保佑一方，为万民祈福。

Yuelu Academy --- One of the four ancient Chinese Academies, conducting research and providing education continuously over 1000 years since 976. Changed into Hunan University in 1926 and it is now the most important part of Hunan University.

岳麓书院：中国古代四大书院之一，历经千年办学不辍，故称"千年学府", 1926年更名为湖南大学。院内环境优美，四季风景如画，古建筑群规模宏大，气势恢弘。碑匾楹联，浩如烟海；圣贤学者，灿若星河。是一处集休闲、旅游、访古、求学于一体的著名文化旅游胜地。

Aiwan Pavilion --- located at breeze gorge of Yuelu Mountain, established in 1792 with
its name derived from the poem "Climbing Yuelu Mountain" by famous poet Du Mu (803-852) of Tang dynasty, in which he depicted vividly a nature beauty when he saw red maple leaves twinkling in nightfall, he had to stop his horse and sat down to enjoy the scenery. Together with Pavilion of Drank, Pavilion of West Lake, Pavilion of Taoran, they are known as the 4 most famous Chinese pavilions. Aiwan Pavilion was also the place where late Chinese leader Chairman Mao liked to stay with his fellow young comrades.  

爱晚亭：位于湖南省岳麓山清风峡中,始建于 1792 年,名字源于杜牧的《山行》: 远上寒山石径斜, 白云生处有 人家。停车坐爱枫林晚, 霜叶红于二月花。爱晚亭与醉翁亭、西湖湖心亭、陶然亭并称中国四大名亭。爱晚亭是毛泽东早年在湖南长沙求学从事革命活动的地方, 为省级文物保护单位。  

The planned time schedule is listed as follows:  

- **13:30-14:00**  Meet in hotel lobby at 13:30 for Kaifu Temple by shuttle bus  
  13:30 酒店大厅集合, 乘车抵达开福寺  
- **14:00-15:00**  Visit Kaifu Temple  
  参观开福寺  
- **15:00-15:40**  Take Eco-friendly bus along Xiangjiang River to Yuelu Academy  
  乘车赴沿江风光带, 而后乘环保车抵达千年学府岳麓书院  
- **15:40-17:00**  Visit Yuelu Academy and Aiwan Pavilion  
  千年学府——岳麓书院、江南四大名亭之首——爱晚亭  
- **17:00-17:30**  Finish the wonderful touring and take shuttle bus back to hotel!  
  游览完后送抵酒店，结束愉快的长沙之旅!
Conference Banquet

In keeping with CALPHAD tradition, the conference banquet will be held at Empark Grand Hotel on Wednesday evening (June 4th). During the banquet, some Chinese shows are planned, and the arrangement is listed as follows:

- **18:00-18:20** Registration (Live Show of Violin)
  来宾签到（现场女子小提琴演奏）

- **18:20-18:25** Opening: Isis Wings Dance
  女子金翅舞开场

- **18:26-18:29** Host
  主持人出场

- **18:30-19:00** (1) Toasts Speech by the President of CSU: Prof. Yaoxue Zhang
  中南大学校长致祝酒词：张尧学教授
  (2) Summary & Prospective of CALPHAD XLIII: Prof. Yong Du (CSU)
  CALPHAD XLIII 的总结与展望：杜勇教授
  (3) CALPHAD Student Scholarship: Prof. Zi-Kui Liu (PSU)
  CALPHAD 学生奖学金颁奖仪式：刘梓葵教授
  (4) STT Student Scholarship: Prof. John Ågren (KTH)
  STT 学生奖学金颁奖仪式：John Ågren 教授
  (5) CALPHAD XLIV in Italy: Prof. Gabriele Cacciamani (UDG)
  第 44 届 CALPHAD 会议情况介绍：Gabriele Cacciamani 教授

- **19:00-19:20** Playing Chinese folk music (Dulcimer & Bamboo & Lute & Erhu)
  中国民乐四连奏（扬琴&竹管&琵琶&二胡）

- **19:20-19:40** Live performance of Kuidi Xu, local Calligrapher
  (His works can be presented to foreign friends with request)
  湖南省书法家协会许魁第大师现场演绎（可现场赠与国际友人）

- **19:40-19:45** Chinese Paper-Cutting
  中国剪纸艺术表演

- **19:45-19:50** Chinese Fan Dance
  中国扇子舞

- **19:50- ...** End of Show, and the banquet continues
  主持人宣布表演结束、晚宴继续
A Few Facts (just in case)

1) Where can I get Internet access?
Free wifi is available in the conference hall and public area of the hotel. Internet access in your room is also provided freely for your laptop via a cable. Please note that if you use the computer in the room it will be charged.

2) Do I need to have my badge with me all the time?
Yes. You will only be permitted to enter the conference hall by displaying a visible badge. If you lose your badge, please go straight to the conference desk with some form of identification where we can make a replacement one for you.

3) How about the weather of Changsha in June?
Weather of Changsha in June is a little bit fickle, thus it is necessary to take an umbrella when you go out in case of rain. The average temperatures from June 1st to 6th in 2011, 2012 and 2013 were 20.7, 21.9 and 26.4 °C, respectively.

4) How can I charge my laptop and other electric appliances?
The electricity supply in China is 220V alternating current at 50Hz. Sockets and plugs are as shown here. We cannot supply enough power adaptors, you’d better prepare one in advance.

5) Emergency call?
Please dial 110 for help from the police, 120 for the ambulance, and 119 for fire emergency.

6) Any suggestions on what to visit after the conference?
Besides those places listed in the social program, there are also some places of interest not too far from Changsha, such as, Zhangjiajie National Park (a one-hour flight from Changsha), which is a 5A-level tourist spots; Fenghuang Ancient City (a five-hour drive from Changsha) if you are interested in the traditional culture in China; Guilin (a three-hour high-speed train from Changsha), with which we have the saying “East or west, Guilin scenery is best”; Beijing (a two-hour fly from Changsha), the capital city, is also a place worth visiting, etc. More information can be found on the official website.

7) Some more tips
(i) Please bring your passport and other valuables with you or put them in the safty box when you leave your room. Be careful when you go across the street, and pay attention to your important items such as passport, bank/credit card and other valuables in public place.
(ii) Please make a copy of your PPT file on the public laptop at least one session before your talk. Our colleague will help you there.
(iii) ... ...
CALPHAD Student Fellowship Awardees

The following is a list of recipients of student fellowship offered by CALPHAD, inc.

(1) Jacob, Aurélie
   Forschungszentrum Juelich, Germany

(2) Zhang, Fan
   Central South University, China

(3) Chen, Yi
   IMDEA Materials Institute, Spain

(4) Yin, Ming
   Illinois Institute of Technology, USA

(5) Kim, Min-Su
   Pohang University of Science and Technology, Republic of Korea

(6) Otis, Richard
   Penn State University, USA

(7) Ouzilleau, Philippe
   École Polytechnique de Montréal, Canada

(8) Wang, Fangfang
   University of Science and Technology Beijing, China

(9) An, Dong
   Southeast University, China

(10) Chizhko, Oleg
     Moscow Environmental Center, Russia
STT Student Fellowship Awardees

The following is a list of recipients of student fellowship offered by the Foundation for Applied Thermodynamics (STT, Stiftelsen för Tillämpad Thermodynamik)

(1) Lin, Chongmao
   Shanghai University, China

(2) Zheng, Weisen
   Shanghai University, China

(3) Li, Zhou
   KTH Royal Institute of Technology, Sweden

(4) Zhou, Bi-Cheng
   Penn State University, USA

(5) Chojnacka, Ida
   Wroclaw University of Technology, Poland

(6) Bigdeli, Sedigheh
   KTH Royal Institute of Technology, Sweden

(7) Zhang, Xi
   Delft University of Technology, The Netherlands

(8) Yang, Yang
   KTH Royal Institute of Technology, Sweden
Session Program

Monday, June 2\textsuperscript{nd}
- Session 1 - Modeling & Software I
- Session 2 - Database Development
- Session 3 - Application of CALPHAD Method I
- Session 4 - CALPHAD Assessments & Experiments I
- Poster Session I (odd numbers)

Tuesday, June 3\textsuperscript{rd}
- Session 5 - Ab Initio I
- Session 6 - Modeling & Software II
- Session 7 - Diffusion
- Session 8 - Microstructure Characterization & Simulation I
- Poster Session II (even numbers)

Wednesday, June 4\textsuperscript{th}
- Session 9 - Ab Initio II
- Session 10 - CALPHAD Assessments & Experiments II

Thursday, June 5\textsuperscript{th}
- Session 11 - Nano, Functional & Energy Materials
- Session 12 - CALPHAD Assessments & Experiments III
- Session 13 - Application of CALPHAD Method II
- Session 14 - CALPHAD Assessments & Experiments IV
- Software Demonstration Session

Friday, June 6\textsuperscript{th}
- Session 15 - CALPHAD Assessments & Experiments V
- Session 16 - Microstructure Characterization & Simulation II
**Monday (Morning), June 2^nd, 2014**

### Welcome remarks (Zhanpeng Jin, Boyun Huang, Yong Du)

大会欢迎辞（金展鹏院士、黄伯云院士、杜勇教授）

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<tr>
<th>Time</th>
<th>Session 1 - Modeling &amp; Software I</th>
</tr>
</thead>
<tbody>
<tr>
<td>08:30</td>
<td><strong>Chairs:</strong> Zi-Kui LIU / Guanghui RAO</td>
</tr>
<tr>
<td></td>
<td>Ågren, John; Larsson, Henrik; Höglund, Lars.</td>
</tr>
<tr>
<td></td>
<td>Thermodynamic and kinetic modelling of internal oxidation</td>
</tr>
<tr>
<td>08:50</td>
<td>[O1] Schmid-Fetzer, Rainer; Milan, Hampl.</td>
</tr>
<tr>
<td></td>
<td>Titanium oxycarbide: modeling approaches in the Ti-C-O system</td>
</tr>
<tr>
<td>09:20</td>
<td>[O2] Lehmann, Jean; Chen, Chunlin; Zhang, Ling.</td>
</tr>
<tr>
<td></td>
<td>What do we do at ArcelorMittal with thermodynamic models?</td>
</tr>
<tr>
<td></td>
<td>The Ag-Pd-Sn and Au-Cu-Sn systems: hard cases for polynomial model?</td>
</tr>
<tr>
<td></td>
<td>A thermodynamic model and database development for molten oxysulfide solutions</td>
</tr>
<tr>
<td>10:30</td>
<td>Coffee break</td>
</tr>
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</table>

### Session 2 - Database Development

<table>
<thead>
<tr>
<th>Time</th>
<th>Session 2 - Database Development</th>
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</thead>
<tbody>
<tr>
<td>10:50</td>
<td><strong>Chairs:</strong> Jan VRESTAL / Xuping SU</td>
</tr>
<tr>
<td></td>
<td>Kang, Youn-Bae; Pelton, Arthur D.; Lee, Hae-Geon.</td>
</tr>
<tr>
<td></td>
<td>A thermodynamic model and database development for molten oxysulfide solutions</td>
</tr>
<tr>
<td>11:10</td>
<td>[O6] Kim, Junghwan; Van Ende, Marie-Aline; Konar, Bikram; Jung, In-Ho.</td>
</tr>
<tr>
<td></td>
<td>Thermodynamic modeling of REE containing systems: Energetics of the REE-X systems (X = Al, Mg, Zn, Sn, Mn, Pb, Fe, Co, Ni)</td>
</tr>
<tr>
<td>11:30</td>
<td>[O7] Kaplan, Bartek; Norgren, Susanne; Schwind, Martin; Selleby, Malin.</td>
</tr>
<tr>
<td></td>
<td>Thermodynamic modeling of Cr-containing cemented carbide materials</td>
</tr>
<tr>
<td></td>
<td>Development of a thermodynamic database for the Na₂O-FeO-Fe₂O₃-SiO₂-S system for the de-sulfurization of molten steel</td>
</tr>
<tr>
<td>12:10</td>
<td>[O9] Wu, Bo; Zhou, Zeyou; Peng, Qiong; Dou, Shushi; Fang, Yuan; Wu, Yufeng; Yang, Shangjii; Wei, Zhenyi; Chen, Zuhua.</td>
</tr>
<tr>
<td></td>
<td>Thermodynamic properties and phase diagram revisit of Al-Sc binary system from ab initio calculations and calphad assessment</td>
</tr>
<tr>
<td>12:30</td>
<td>Lunch</td>
</tr>
</tbody>
</table>
### Monday (Afternoon), June 2nd

#### Session 3 - Application of CALPHAD Method I

**Chairs:** John ÅGREN / Lin LI

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker(s)</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>14:00</td>
<td>Ishida, K.</td>
<td>Thermodynamic Database, Alloy Design and Industrial Applications of Cu-based Alloys</td>
</tr>
<tr>
<td>14:30</td>
<td>Luo, Alan A.</td>
<td>Integrated Computational Materials Engineering (ICME) for Light Metals and Manufacturing</td>
</tr>
<tr>
<td>14:50</td>
<td>Schneider, André; Köster, Aenne.</td>
<td>Application of the CALPHAD method for seamless tubes and pipes</td>
</tr>
<tr>
<td>15:10</td>
<td>Gong, Jiadong; Snyder, David; Sebastian, Jason; Olson, Greg.</td>
<td>Computational Design of a Novel Co-Base Alloy for Cu-Be Replacement</td>
</tr>
<tr>
<td>15:30</td>
<td>Wang, Kang; Wang, Haifeng; Liu, Feng.</td>
<td>Application of maximum entropy production principle to rapid solidification</td>
</tr>
</tbody>
</table>

**Coffee break**

### Session 4 - CALPHAD Assessments & Experiments I

**Chairs:** Rainer SCHMID-FETZER / Fucheng YIN

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker(s)</th>
<th>Title</th>
</tr>
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<tbody>
<tr>
<td>16:10</td>
<td>Lepple, Maren; Cupid, Damian M.; Franke, Peter; Seifert, Hans J.</td>
<td>Thermodynamic modeling and experimental investigations of materials systems for lithium-ion batteries</td>
</tr>
<tr>
<td>16:40</td>
<td>Povoden-Karadeniz, Erwin; Moszner, Frank; Pogatscher, Stefan; Uggowitzer, Peter J; Kozeschnik, Ernst.</td>
<td>Thermodynamics of the Pd-Mn system and phase stability of L10-based Pd1_xMn1_yFe_x+y.</td>
</tr>
<tr>
<td>17:00</td>
<td>Li, Dongdong; Zeng, Dewen; Yin, Xia; Han, Haijun.</td>
<td>Thermodynamic modeling of Salt Lake Brine System: Parameterization Strategy</td>
</tr>
<tr>
<td>17:20</td>
<td>Zhang, Shuai; Jiang, Min; Li, Hongxiao; Ren, Yuping; Wang, Lei; Qin Gaowu.</td>
<td>Thermodynamic calculation of the Mg-Cu-Y system</td>
</tr>
<tr>
<td>17:40</td>
<td>Li, Dajian; Fürtauer, Siegfried; Flandorfer, Hans; Cupid, Damian M.</td>
<td>Recent progress of thermodynamic study with Sn based anode materials for Li-ion battery application</td>
</tr>
</tbody>
</table>

**Dinner**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker(s)</th>
<th>Title</th>
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<tbody>
<tr>
<td>19:30</td>
<td></td>
<td>Poster Session I (odd numbers)</td>
</tr>
</tbody>
</table>

**Chairs:** Cacciamani GABREILE / Min JIANG
### Tuesday (Morning), June 3rd

#### Session 5 - Ab Initio I

**Chairs:** Byeong-Joo LEE / Jianyun SHEN

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Details</th>
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</thead>
<tbody>
<tr>
<td>08:30 [O20]</td>
<td>Liu, Zi-Kui. Entropy</td>
</tr>
<tr>
<td>09:00 [O21]</td>
<td>Neugebauer, Jörg; Todorova, Mira. Connecting thermodynamic concepts of semiconductor defect chemistry with electrochemistry</td>
</tr>
<tr>
<td>09:30 [O22]</td>
<td>Huang, Guoxing; Zeng, Lijun; Wang, Xing; Liu, Libin. First-principles calculations of point defects in B2 phase</td>
</tr>
<tr>
<td>10:30</td>
<td>Coffee break</td>
</tr>
</tbody>
</table>

#### Session 6 - Modeling & Software II

**Chairs:** Alan LUO / Xianran XING

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Details</th>
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</thead>
<tbody>
<tr>
<td>10:50 [O25]</td>
<td>Sundman, Bo, Chen, Qing. A database format for integrated computational materials engineering</td>
</tr>
<tr>
<td>11:10 [O26]</td>
<td>Chartrand, Patrice; Robelin, Christian; Gemme, Frédéric. A thermodynamic model for the NH$_4^+$, K$^+$ // H$_2$PO$_4^-$, H$_2$P$_2$O$_7^{2-}$, NO$_3^-$, Cl$^-$ - H$_2$O system for fertilizer applications</td>
</tr>
<tr>
<td>11:30 [O27]</td>
<td>Chen, Qing; Wu, Kaisheng; Mason, Paul; Bratberg, Johan; Engström, Anders. Prediction of precipitate microstructures with a CALPHAD-based computational tool</td>
</tr>
<tr>
<td>11:50 [O28]</td>
<td>Zhang, Fan; Cao, Weisheng; Chen, Shuanglin; Zhang, Chuan; Zhu, Jun. Beyond Phase Diagrams: Precipitation Simulation of Multicomponent Alloys by the CALPHAD Approach</td>
</tr>
<tr>
<td>12:10 [O29]</td>
<td>Du, Qiang; Li, Y.J.; Tang, Kai. As cast grain size prediction via CALPHAD and CALPHAD-coupled kinetic approaches</td>
</tr>
<tr>
<td>12:30</td>
<td>Lunch</td>
</tr>
</tbody>
</table>

19
Tuesday (Afternoon), June 3rd

Session 7 - Diffusion

Chairs: Jörg NEUGEBAUER / Lixian SUN

Design of sustainable V-based hydrogen separation membranes based on grain boundary segregation

14:30 [O31] Chang, Keke; Music, Denis; Lange, Dennis; to Baben, Moritz; Bolvardi, Hamid; Schneider, Jochen M.
Estimating metastable phase formation during magnetron sputtering

14:50 [O32] Voytovych, Rayisa; Hodaj, Fiqiri; Cornu, Marie-José; Koltsov, Alexey; Pesci, Cécile.
Thermodynamics and kinetics of interfacial interactions between oxide layer on a steel surface and liquid Na₂O-SiO₂-B₂O₃-TiO₂ glass

15:10 [O33] Naraghi, Reza; Höglund, Lars; Ågren, John.
Application of compound-energy formalism to the parabolic growth of solid metal oxides

15:30 [O34] Zhang, Lijun; Chen, Qing.
Revisiting the phenomenological model for effect of chemical ordering on diffusion

15:50 Coffee break

Session 8 - Microstructure Characterization & Simulation I

Chairs: Hans J. SEIFERT / Yifang OUYANG

16:10 [O35] Zhu, Mingfang; Dai, Ting; Cao, Weisheng; Chen, Shuanglin.
Modeling of dendritic microstructure and microsegregation in solidification of Al-rich multi-component alloys

16:40 [O36] Stratmann, Matthias; Zhang, Lijun; Shchyglo, Oleg; Steinbach, Ingo.
Phase-field simulation of precipitation using the CALPHAD sublattice approach and thermodynamic databases

17:00 [O37] Ni, Y.; Zhang, L.; Lu, YY; Song, Y.C.
Evolution of diffusion induced stress in phase separating electrodes

17:20 [O38] Iseya, Kenji; Mimura, Kenshiro; Miura, Seiji; Mohri, Tetsuo.
Evaluation of Phase Field Image based on CVM and Spectral analysis

17:40 [O39] Xie, Yu; Dong, Hongbiao.
Modelling of solidification structure evolution and solute segregation in a weld pool using a multi-scale approach

18:00 [O40] Cui, Yuwen; Xu, Guanglong; Lee, Dong-Wook.
Integrated Landau Model of Martensite in Steels and Shape Memory Alloys

18:20 Dinner

19:30 - 21:30 Poster Session II (even numbers)
Chairs: Ikuo OHNUMA / Yuqin LIU
### Session 9 - Ab Initio II

**Chairs:** Ernst KOZESCHNIK / Mingfang ZHU

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker(s)</th>
<th>Title</th>
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<tbody>
<tr>
<td>08:30</td>
<td>Chen, Xing-Qiu; Cheng, Xiyue; Niu, Haiyang.</td>
<td>Missing aspects in the structural phases of TMB₄ tetraborides (TM = Cr and W): First-principles calculations and experimental verifications</td>
</tr>
<tr>
<td>08:50</td>
<td>Bai, Kewu; Tan, Teck Leoeng; Branicio, Paulo Sergio; Sullivan, Michael.</td>
<td>Crystallization kinetic studies of GeSbTe phase change materials by ab initio molecular dynamics</td>
</tr>
<tr>
<td>09:10</td>
<td>Hickel, T.; Glensk, A.; Körmann, F.; Grabowski, B.; Bleskov, I.; Neugebauer, J.</td>
<td>Ab initio description of thermodynamic properties in unaries: A progress report</td>
</tr>
<tr>
<td>09:30</td>
<td>Guo, Zifeng; Wang, Ziru; Lan, Chunxiang; Tao, Xiaoma; Ouyang, Yifang.</td>
<td>Phase stability, electronic and mechanical properties of NaCl-type RMₓAl₁₋ₓN (RM = Ta, Mo and W) from first-principles calculations</td>
</tr>
<tr>
<td>09:50</td>
<td>Song, Qi; Jiang, Zhen-Yi; Zhang, Zhi-Yong; Zhan, Xiao-Dong.</td>
<td>From orientation disordered to ordered—an ab initio simulation on Ammonia Borane phase transition within van der Waals corrections</td>
</tr>
<tr>
<td>10:10</td>
<td>Tsai, Ping-chun; Hsu, Wen-Dung; Lin, Shih-kang.</td>
<td>Ab initio-aided defect spinel electrode design for lithium ion batteries with high cyclability</td>
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<th>Time</th>
<th>Notes</th>
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<tr>
<td>10:30</td>
<td>Coffee break</td>
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</tbody>
</table>

### Session 10 - CALPHAD Assessments & Experiments II

**Chairs:** Tomas GOMEZ-ACEBO / In-Ho JUNG

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker(s)</th>
<th>Title</th>
</tr>
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<tbody>
<tr>
<td>10:50</td>
<td>Chen, Sinn-wen; Wu, Hsin-jay.</td>
<td>Phase equilibria of thermoelectric materials: Ag-Sb-Te and AgSbTe₂-AgSbSe₂</td>
</tr>
<tr>
<td>11:20</td>
<td>Vřešťál, Jan; Pavlí, Jana; Wdowik, Urszula, D.; Šob, Mojmir.</td>
<td>Thermodynamic modeling below room temperature: Hf-V system</td>
</tr>
<tr>
<td>11:40</td>
<td>Kaptay, George; Mekler Csaba; Vegh, Adam.</td>
<td>CALPHAD - compatible models for interfacial energies</td>
</tr>
<tr>
<td>12:00</td>
<td>Shinagawa, Kazuya; Chinen, Hibiki; Omori, Toshihiro; Oikawa, Katsunari; Ohnuma, Ikuo; Ishida, Kiyohito; Kainuma, Ryosuke.</td>
<td>Phase equilibria and thermodynamic evaluation of the Co-Ta binary system</td>
</tr>
<tr>
<td>12:20</td>
<td>Yin, Ming; Nash, Philip.</td>
<td>Standard enthalpies of formation of half-Heusler compounds XYSn (X = Au, Co, Fe, Ir, Ni, Pd, Pt; Y = Hf, Mn, Ti, V, Zr)</td>
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<tr>
<th>Time</th>
<th>Notes</th>
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<tbody>
<tr>
<td>12:40</td>
<td>Lunch</td>
</tr>
<tr>
<td>13:30</td>
<td>Conference excursion: Kaifu Temple (开福寺), Yuelu Academy (岳麓书院) and Aiwan Pavilion (爱晚亭)</td>
</tr>
<tr>
<td>18:00</td>
<td>Conference Banquet: Empark Grand Hotel (世纪金源大饭店)</td>
</tr>
</tbody>
</table>
### Thursday (Morning), June 5th

**Session 11 - Nano, Functional & Energy Materials**

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
</table>
| 08:30 | Song, Xiaoyan; Zhou, Yuanyuan; He, Jiangtao; Xu, Wenwu; Wang, Haibin; Liu, Xuemei.  
Phase stability in nanocrystalline partially ionic solids |
| 08:50 | Lee, Joonho; Sim, Kijoo.  
Prediction of the phase diagram of Sn-Ag nanoparticles |
| 09:10 | Gasiór, Władysław; Polański, Marek; Pstruś, Janusz; Dębski Adam.  
Studies on hydrogen storage materials from the Li-B and Ca-Li systems |
| 09:30 | Saengdeejing, Arkapol; Chen, Ying; Suzuki, Ken; Miura, Hideo; Matsuura, Masashi; Sugimoto, Satoshi.  
Studies on hydrogen storage materials from the Li-B and Ca-Li systems |
| 09:50 | Kim, Na Rae; Shin, Kihyun; Lee, Hyuck Mo.  
Fabrication of Ag-Cu Nanoparticles Based on the Nano-Phase Diagram and Anti-Oxidation Effects |
| 10:10 | Wang, Fangfang; Xie, Ying; Chen, Jun; Fu, Honggang; Xing, Xianran.  
First-principles study on negative thermal expansion of PbTiO3 |
| 10:30 | **Coffee break** |

### Session 12 - CALPHAD Assessments & Experiments III

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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</thead>
</table>
The isothermal section of the Nd-Mn-As phase diagram at 500 °C and 800 °C |
| 11:10 | Yin, Fucheng; Wang, Weilin; Zhao, Maoxiu; Li, Zhi; Wu, Yu.  
Experimental investigation and thermodynamic calculation of the Co-Si-Zn system |
| 11:30 | Rajagopal, Anand; Århammar, Cecilia; Holmström, Erik; Ojha, Rohit; Zhang, Hui; Sahlberg, Martin; Norgren, Susanne.  
On oxygen content and phase equilibria in the Ti-Al binary system |
| 11:50 | Li, Shuai; Xie, Wei; Qiao, Zhiyu; Cao, Zhanmin.  
Critical evaluation and thermodynamic optimization of the V-O system |
| 12:10 | He, Cuiyun; Sun, Songxiang; Zhou, Hua; Wang, Peisheng; Du, Yong.  
Experimental investigation and thermodynamic assessment of the Ca-Y, Mg-Ca-Y, Ce-Sr and Mg-Ce-Sr systems |
| 12:30 | **Lunch** |
**Session 13 - Application of CALPHAD Method II**

<table>
<thead>
<tr>
<th>Time</th>
<th>Presentation</th>
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</thead>
<tbody>
<tr>
<td>13:50</td>
<td>Zhong, Yu; Yang, Mei; Chen, Ming. Application of computational thermodynamics in solid oxide fuel cell</td>
</tr>
<tr>
<td>14:10</td>
<td>Wang, Jianwei; Wang, Lijun; Wang, Ligen; Huang, Guojie; Cheng, Lei; Xiao, Wei. Application of CALPHAD method on the cracking control of Nb-containing bulk zirconium hydride</td>
</tr>
<tr>
<td>14:30</td>
<td>Li, Lin; Gao, Yi; He, Yanlin; Shi, Wen; Zhang, Mei; Lu, Xiaogang. Optimization of mechanical properties of high strength TRIP steels</td>
</tr>
<tr>
<td>14:50</td>
<td>Chizhko, Oleg. Thermodynamic modeling of crystal structures for high-temperature anti-corrosion coatings</td>
</tr>
<tr>
<td>15:10</td>
<td>Brosh, Eli. Modeling of the thermophysical properties of Fe-Ni alloys with application to calculation of high-pressure phase equilibria</td>
</tr>
<tr>
<td>15:30</td>
<td>Luo, Qun; Li, Qian; Zhang, Jie-Yu; Chou, Kuo-Chih. Comparison of Muggianu model, Toop model and General solution model for predicting the thermodynamic properties of Mg-Al-Zn system</td>
</tr>
<tr>
<td>15:50</td>
<td>Coffee break</td>
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**Session 14 - CALPHAD Assessments & Experiments IV**

<table>
<thead>
<tr>
<th>Time</th>
<th>Presentation</th>
</tr>
</thead>
<tbody>
<tr>
<td>16:10</td>
<td>Zhou, S.H.; Kramer, M.J.; Ott, R.T.; Napolitano, R.E. Energetic investigation of metastable Al$<em>{60}$Sm$</em>{11}$-ω, Al$<em>{5}$Sm-π, Al$</em>{4}$Sm-γ, Al$<em>{1}$Sm$</em>{3}$-α and Al$_{5}$Sm-β phase formation</td>
</tr>
<tr>
<td>16:30</td>
<td>Roslyakova, Irina; Sundman, Bo; Dette, Holger. Modeling of thermo-physic properties for pure elements using segmented regression methodology</td>
</tr>
<tr>
<td>16:50</td>
<td>Broz, Pavel; Zelenka, Frantisek; Vřeštálek, Jan; Bursik, Jiri; Zeiringer, Isolde; Falmbigl, Matthias; Rogl, Gerda; Rogl, Peter Franz. Study of thermal stability of advanced thermoelectrics by means of thermal analysis and Knudsen effusion mass spectrometry</td>
</tr>
<tr>
<td>17:10</td>
<td>Nuta, Ioana; Chatillon, Christian; Collas, Hervé; Artaud, Laurent; Guetta, Veronique; Heuer, Daniel. Vapor pressure measurements of LiF-ZrF$_4$ for Molten Salt Fast Reactor</td>
</tr>
<tr>
<td>17:30</td>
<td>Tang, Chengying; Shen, Wei; Xu, Wei; Wang, Jiang; Zhou, Huaiying. Size-dependent eutectic melting and thermodynamic properties of Ag-Cu alloy nanoparticles</td>
</tr>
<tr>
<td>17:50</td>
<td>Liu, Ya; Li, Daiyu; Su, Xuping; Wang, Jianhua. Microstructure differences and formation mechanisms of periodic-layered structure in Ni$_3$Si/Zn system with Zn in vapor or liquid state</td>
</tr>
<tr>
<td>18:10</td>
<td>Dinner</td>
</tr>
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</table>
**Software Demonstration Session**

**Thursday (Evening), June 5th**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker(s)</th>
<th>Topic</th>
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</thead>
<tbody>
<tr>
<td>19:30</td>
<td>Chen, Qing; Kjellqvist, Lina.</td>
<td>Thermo-Calc, DICTRA, and TC-PRISMA - A Continuing Integration</td>
</tr>
<tr>
<td>20:00</td>
<td>Zhang, Fan.</td>
<td>PANDAT software for multi-component phase equilibrium calculation and precipitation simulation</td>
</tr>
<tr>
<td>20:30</td>
<td>Chartrand, Patrice; Jung, In-Ho.</td>
<td>Recent development of FactSage software and database</td>
</tr>
<tr>
<td>21:00</td>
<td>Effenberg, Günter.</td>
<td>MSI Eureka: Best practice for projects and CALPHAD</td>
</tr>
<tr>
<td>21:30</td>
<td>Sundman, Bo.</td>
<td>Open Calphad Software</td>
</tr>
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</table>
**Friday (Morning), June 6th**

### Session 15 - CALPHAD Assessments & Experiments V

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
</tr>
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<tbody>
<tr>
<td>08:30</td>
<td>075 Phase projection diagrams</td>
<td>Chen, Shuanglin; Cao, Weisheng; Zhang, Fan; Zhang, Chuan; Zhu, Jun; Schmid-Fetzer, Rainer; Li, Qian; Zhang, Jieyu</td>
</tr>
<tr>
<td>09:10</td>
<td>077 The reassessment of the Al-Cu and Cu-Zn systems with respect to the γ-brass phase</td>
<td>Kroupa, A.; Vrestal, J.; Boulet, Pascal; Dinsdale, A.; Watson, A.; Record, M.-Ch.</td>
</tr>
<tr>
<td>09:30</td>
<td>078 Ternary phase diagram studies of Orientationally Disordered “Plastic Crystals”</td>
<td>Chandra, Dhanesh; Mishra, Amrita; Shi, Renhai; Talekar, Anjali.</td>
</tr>
<tr>
<td>09:50</td>
<td>079 The isothermal section of the phase diagram of Gd-Fe-Mn system at 773 K</td>
<td>Ma, Ruting; He, Wei.</td>
</tr>
<tr>
<td>10:10</td>
<td>080 Thermodynamic modeling of Ti-Fe-Mn ternary system</td>
<td>Hu, Renmin; He, Jin; Zhou, Han; Lu, Xionggang; Li, Chonghe.</td>
</tr>
<tr>
<td>10:30</td>
<td>Coffee break</td>
<td></td>
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</table>

### Session 16 - Microstructure Characterization & Simulation II

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:50</td>
<td>081 Study on formation mechanism of difference structures of ZrO₂ as Zr corrosion products</td>
<td>Shen, Jianyun; Zhao, Xushan; Feng, Xuankai; Yuan, Gaihuan; Yue, Qiang.</td>
</tr>
<tr>
<td>11:10</td>
<td>082 Icosahedral-decahedral transformation in the Pd-Ag bimetallic cluster induced by Ag atomic segregation</td>
<td>Li, Guojian; Wang, Kai; Du, Jiaojiao; Wang, Qiang.</td>
</tr>
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<td>11:30</td>
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