



## **PROGRAM BOOKLET**

Computer Coupling of Phase Diagrams and  
Thermochemistry

### **CALPHAD XLIII**

June 1<sup>st</sup> to June 6<sup>th</sup>, 2014

Changsha, Hunan, CHINA

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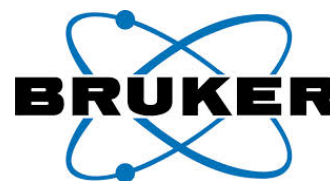
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The Foundation for Applied Thermodynamics (STT)



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## **CALPHAD XLIII**

Central South University, Changsha  
June 1-6, 2014  
Changsha, China



## **SOCIAL PROGRAM (for accompanying people)**

### **Sunday, June 1<sup>st</sup>**

- 19:30 Welcome cocktail at Empark Grand Hotel

### **Monday, June 2<sup>nd</sup>**

- 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<sup>rd</sup>**

- 08:30 Go to Yueyang City, and visit Yueyang Pavilion
- 10:30 Visit Sanzui Pavilion, Xianmei Pavilion, Xiaoqiao 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<sup>th</sup>**

- 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<sup>th</sup>**

- 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<sup>th</sup>**

- 13:00 Lunch at Empark Grand Hotel

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## Program at a Glance

	June 1 <sup>st</sup> (Sun)	June 2 <sup>nd</sup> (Mon)	June 3 <sup>rd</sup> (Tue)	June 4 <sup>th</sup> (Wed)	June 5 <sup>th</sup> (Thu)	June 6 <sup>th</sup> (Fri)
8:30	Welcome	8:30 Welcome	8:30	8:30	8:30	8:30
9:00		8:50	S5: Ab initio (I)	S9: Ab initio (II)	S11: Nano, Functional, & Energy Materials	S15: CALPHAD Assessment & Experiment (V)
9:30		S1: Modeling & Software (I)				
10:00						
10:30		10:30	10:30	10:30	10:30	10:30
11:00		Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
11:30		10:50	10:50	10:50	10:50	10:50
12:00		S2: Database Development	S6: Modeling & Software (II)	S10: CALPHAD Assessment & Experiment (II)	S12: CALPHAD Assessment & Experiment (III)	S16: Microstructure Characterization & Simulation (II)
12:30		12:30	12:30	12:40	12:30	12:30
13:00		Lunch	Lunch	Lunch	Lunch	12:30 Closing Session
13:30			13:30		13:00 Lunch	
14:00	14:00	14:00	Conference Excursion	13:50		
14:30	S3: Application of CALPHAD method (I)	S7: Diffusion		13:50		S13: Application of CALPHAD method (II)
15:00				15:50		
15:30	15:50	15:50		15:50		
16:00	Coffee break	Coffee break		Coffee break		
16:30	16:10	16:10		16:10		
17:00	S4: CALPHAD Assessment & Experiment (I)	S8: Microstructure Characterization & Simulation (I)		S14: CALPHAD Assessment & Experiment (IV)		
17:30						
18:00	18:00	18:20	18:30	18:10		
18:30	Dinner	Dinner	Conference Banquet	Dinner		
19:00						
19:30	19:30	19:30		19:30		
20:00	19:30 Welcome Cocktail	Poster Session I (odd numbers)	Poster Session II (even numbers)	Software Demonstration Session		
20:30						

## 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 4<sup>th</sup>, 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, 古建筑群规模庞大, 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

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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

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In keeping with CALPHAD tradition, the conference banquet will be held at Empark Grand Hotel on Wednesday evening (June 4<sup>th</sup>). 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)

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### 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 at all times?

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 1<sup>st</sup> to 6<sup>th</sup> 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 safety 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**

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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**

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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**

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### **Monday, June 2<sup>nd</sup>**

- 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<sup>rd</sup>**

- 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<sup>th</sup>**

- Session 9 - Ab Initio II
- Session 10 - CALPHAD Assessments & Experiments II

### **Thursday, June 5<sup>th</sup>**

- 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<sup>th</sup>**

- Session 15 - CALPHAD Assessments & Experiments V
- Session 16 - Microstructure Characterization & Simulation II



**Monday (Morning), June 2<sup>nd</sup>**

08:30	<b>Welcome remarks</b> (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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**Session 1 - Modeling & Software I**

<b>Chairs: Zi-Kui LIU / Guanghui RAO</b>	
08:50 [O1]	<u>Ågren, John</u> ; Larsson, Henrik; Höglund, Lars. Thermodynamic and kinetic modelling of internal oxidation
09:20 [O2]	<u>Schmid-Fetzer, Rainer</u> ; Milan, Hampl. Titanium oxycarbide: modeling approaches in the Ti-C-O system
09:50 [O3]	<u>Lehmann, Jean</u> ; Chen, Chunlin; Zhang, Ling. What do we do at ArcelorMittal with thermodynamic models?
10:10 [O4]	<u>Kuznetsov, Viktor N.</u> ; Kabanova, Elizaveta G. The Ag-Pd-Sn and Au-Cu-Sn systems: hard cases for polynomial model?
10:30	<b>Coffee break</b>

**Session 2 - Database Development**

<b>Chairs: Jan VRESTAL / Xuping SU</b>	
10:50 [O5]	<u>Kang, Youn-Bae</u> ; Pelton, Arthur D.; Lee, Hae-Geon. A thermodynamic model and database development for molten oxysulfide solutions
11:10 [O6]	Kim, Junghwan; Van Ende, Marie-Aline; Konar, Bikram; <u>Jung, In-Ho</u> . Thermodynamic modeling of REE containing systems: Energetics of the REE-X systems (X = Al, Mg, Zn, Si, Sn, Mn, Pb, Fe, Co, Ni)
11:30 [O7]	<u>Kaplan, Bartek</u> ; Norgren, Susanne; Schwind, Martin; Selleby, Malin. Thermodynamic modeling of Cr-containing cemented carbide materials
11:50 [O8]	<u>Elmira, Moosavi-Khoonsari</u> ; Jung, In-Ho. Development of a thermodynamic database for the Na <sub>2</sub> O-FeO-Fe <sub>2</sub> O <sub>3</sub> -SiO <sub>2</sub> -S system for the de-sulfurization of molten steel
12:10 [O9]	<u>Wu, Bo</u> ; Zhou, Zeyou; Peng, Qiong; Dou, Shushi; Fang, Yuan; Wu, Yufeng; Yang, Shangjin; Wei, Zhenyi; Chen, Zuhua. Thermodynamic properties and phase diagram revisit of Al-Sc binary system from ab initio calculations and calphad assessment
12:30	<b>Lunch</b>

**Monday (Afternoon), June 2<sup>nd</sup>**

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

<b>Chairs: John ÅGREN / Lin LI</b>	
14:00 [O10]	<u>Ishida, K.</u> Thermodynamic Database, Alloy Design and Industrial Applications of Cu-based Alloys
14:30 [O11]	<u>Luo, Alan A.</u> Integrated Computational Materials Engineering (ICME) for Light Metals and Manufacturing
14:50 [O12]	<u>Schneider, André; Köster, Aenne.</u> Application of the CALPHAD method for seamless tubes and pipes
15:10 [O13]	<u>Gong, Jiadong; Snyder, David; Sebastian, Jason; Olson, Greg.</u> Computational Design of a Novel Co-Base Alloy for Cu-Be Replacement
15:30 [O14]	<u>Wang, Kang; Wang, Haifeng; Liu, Feng.</u> Application of maximum entropy production principle to rapid solidification
15:50	<b>Coffee break</b>

**Session 4 - CALPHAD Assessments & Experiments I**

<b>Chairs: Rainer SCHMID-FETZER / Fucheng YIN</b>	
16:10 [O15]	<u>Lepple, Maren; Cupid, Damian M.; Franke, Peter; Seifert, Hans J.</u> Thermodynamic modeling and experimental investigations of materials systems for lithium-ion batteries
16:40 [O16]	<u>Povoden-Karadeniz, Erwin; Moszner, Frank; Pogatscher, Stefan; Uggowitzner, Peter J; Kozeschnik, Ernst.</u> Thermodynamics of the Pd-Mn system and phase stability of L1 <sub>0</sub> -based Pd <sub>1-x</sub> Mn <sub>1-y</sub> Fe <sub>x+y</sub> .
17:00 [O17]	<u>Li, Dongdong; Zeng, Dewen; Yin, Xia; Han, Haijun.</u> Thermodynamic modeling of Salt Lake Brine System: Parameterization Strategy
17:20 [O18]	<u>Zhang, Shuai; Jiang, Min; Li, Hongxiao; Ren, Yuping; Wang, Lei; Qin Gaowu.</u> Thermodynamic calculation of the Mg-Cu-Y system
17:40 [O19]	<u>Li, Dajian; Fürtauer, Siegfried; Flandorfer, Hans; Cupid, Damian M.</u> Recent progress of thermodynamic study with Sn based anode materials for Li-ion battery application
18:00	<b>Dinner</b>
19:30 - 21:30	<b>Poster Session I (odd numbers)</b> <b>Chairs: Cacciamani GABREILE / Min JIANG</b>

**Tuesday (Morning), June 3<sup>rd</sup>**

**Session 5 - Ab Initio I**

<b>Chairs: Byeong-Joo LEE / Jianyun SHEN</b>	
08:30 [O20]	<u>Liu, Zi-Kui.</u> Entropy
09:00 [O21]	<u>Neugebauer, Jörg;</u> Todorova, Mira. Connecting thermodynamic concepts of semiconductor defect chemistry with electrochemistry
09:30 [O22]	Huang, Guoxing; Zeng, Lijun; Wang, Xing; <u>Liu, Libin.</u> First-principles calculations of point defects in B2 phase
09:50 [O23]	<u>Ohtani, Hiroshi;</u> Iikubo, Satoshi. Reexamination of Thermodynamic Properties of Cementite Considering its Nonstoichiometry
10:10 [O24]	<u>Trybula, M.;</u> Jakse, N.; Gancarz, T.; Gąsior, W.; Pasturel, A. Thermodynamic and thermo-physical properties of liquid Al-Li alloys. Molecular dynamics and CFM study vs. experiment
10:30	<b>Coffee break</b>

**Session 6 - Modeling & Software II**

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

**Tuesday (Afternoon), June 3<sup>rd</sup>**

**Session 7 - Diffusion**

<b>Chairs: Jörg NEUGEBAUER / Lixian SUN</b>	
14:00 [O30]	Ko, Won-Seok; <u>Lee, Byeong-Joo</u> . Design of sustainable V-based hydrogen separation membranes based on grain boundary segregation
14:30 [O31]	<u>Chang, Keke</u> ; Music, Denis; Lange, Dennis; to Baben, Moritz; Bolvardi, Hamid; Schneider, Jochen M. Estimating metastable phase formation during magnetron sputtering
14:50 [O32]	Voytovych, Rayisa; <u>Hodaj, Figiri</u> ; Cornu, Marie-José; Koltsov, Alexey; Pesci, Cécile. Thermodynamics and kinetics of interfacial interactions between oxide layer on a steel surface and liquid Na <sub>2</sub> O-SiO <sub>2</sub> -B <sub>2</sub> O <sub>3</sub> -TiO <sub>2</sub> glass
15:10 [O33]	<u>Naraghi, Reza</u> ; Höglund, Lars; Ågren, John. Application of compound-energy formalism to the parabolic growth of solid metal oxides
15:30 [O34]	<u>Zhang, Lijun</u> ; Chen, Qing. Revisiting the phenomenological model for effect of chemical ordering on diffusion
15:50	<b>Coffee break</b>

**Session 8 - Microstructure Characterization & Simulation I**

<b>Chairs: Hans J. SEIFERT / Yifang OUYANG</b>	
16:10 [O35]	<u>Zhu, Mingfang</u> ; Dai, Ting; Cao, Weisheng; Chen, Shuanglin. Modeling of dendritic microstructure and microsegregation in solidification of Al-rich multi-component alloys
16:40 [O36]	<u>Stratmann, Matthias</u> ; Zhang, Lijun; Shchyglo, Oleg; Steinbach, Ingo. Phase-field simulation of precipitation using the CALPHAD sublattice approach and thermodynamic databases
17:00 [O37]	<u>Ni, Y.</u> ; Zhang, L.; Lu, Y.Y.; Song, Y.C. Evolution of diffusion induced stress in phase separating electrodes
17:20 [O38]	Iseya, Kenji; Mimura, Kenshiro; Miura, Seiji; <u>Mohri, Tetsuo</u> . Evaluation of Phase Field Image based on CVM and Spectral analysis
17:40 [O39]	Xie, Yu; <u>Dong, Hongbiao</u> . Modelling of solidification structure evolution and solute segregation in a weld pool using a multi-scale approach
18:00 [O40]	<u>Cui, Yuwen</u> ; Xu, Guanglong; Lee, Dong-Wook. Integrated Landau Model of Martensite in Steels and Shape Memory Alloys
18:20	<b>Dinner</b>
19:30 - 21:30	<b>Poster Session II (even numbers)</b> <b>Chairs: Ikuo OHNUMA / Yuqin LIU</b>

**Wednesday (Morning), June 4<sup>th</sup>**

**Session 9 - Ab Initio II**

<b>Chairs: Ernst KOZESCHNIK / Mingfang ZHU</b>	
08:30 [O41]	<u>Chen, Xing-Qiu</u> ; Cheng, Xiyue; Niu, Haiyang. Missing aspects in the structural phases of TMB <sub>4</sub> tetraborides (TM = Cr and W): First-principles calculations and experimental verifications
08:50 [O42]	<u>Bai, Kewu</u> ; Tan, Teck Leoeng; Branicio, Paulo Sergio; Sullivan, Michael. Crystallization kinetic studies of GeSbTe phase change materials by ab initio molecular dynamics
09:10 [O43]	<u>Hickel, T.</u> ; Glensk, A.; Körmann, F.; Grabowski, B.; Bleskov, I.; Neugebauer, J. Ab initio description of thermodynamic properties in unaries: A progress report
09:30 [O44]	Guo, Zifeng; Wang, Ziru; Lan, Chunxiang; <u>Tao, Xiaoma</u> ; Ouyang, Yifang. Phase stability, electronic and mechanical properties of NaCl-type RMxAl <sub>1-x</sub> N (RM = Ta, Mo and W) from first-principles calculations
09:50 [O45]	Song, Qi; <u>Jiang, Zhen-Yi</u> ; Zhang, Zhi-Yong; Zhan, Xiao-Dong. From orientation disordered to ordered-an ab initio simulation on Ammonia Borane phase transition within van der Waals corrections
10:10 [O46]	Tsai, Ping-chun; Hsu, Wen-Dung; <u>Lin, Shih-kang</u> . Ab initio-aided defect spinel electrode design for lithium ion batteries with high cyclability
10:30	<b>Coffee break</b>

**Session 10 - CALPHAD Assessments & Experiments II**

<b>Chairs: Tomas GOMEZ-ACEBO / In-Ho JUNG</b>	
10:50 [O47]	<u>Chen, Sinn-wen</u> ; Wu, Hsin-jay. Phase equilibria of thermoelectric materials: Ag-Sb-Te and AgSbTe <sub>2</sub> -AgSbSe <sub>2</sub>
11:20 [O48]	<u>Vřešťál, Jan</u> ; Pavlů, Jana; Wdowik, Urszula, D.; Šob, Mojmír. Thermodynamic modeling below room temperature: Hf-V system
11:40 [O49]	<u>Kaptay, George</u> ; Mekler Csaba; Vegh, Adam. Calphad - compatible models for interfacial energies
12:00 [O50]	Shinagawa, Kazuya; Chinen, Hibiki; Omori, Toshihiro; Oikawa, Katsunari; <u>Ohnuma, Ikuo</u> ; Ishida, Kiyohito; Kainuma, Ryosuke. Phase equilibria and thermodynamic evaluation of the Co-Ta binary system
12:20 [O51]	<u>Yin, Ming</u> ; Nash, Philip. Standard enthalpies of formation of half-Heusler compounds XYSn (X = Au, Co, Fe, Ir, Ni, Pd, Pt; Y = Hf, Mn, Ti, V, Zr)
12:40	<b>Lunch</b>
13:30	<b>Conference excursion: Kaifu Temple (开福寺), Yuelu Academy (岳麓书院) and Aiwan Pavilion (爱晚亭)</b>
18:00	<b>Conference Banquet: Empark Grand Hotel (世纪金源大饭店)</b>

**Thursday (Morning), June 5<sup>th</sup>**

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

<b>Chairs: Philip NASH / Jialin YAN</b>	
08:30 [O52]	<u>Song, Xiaoyan</u> ; Zhou, Yuanyuan; He, Jiangtao; Xu, Wenwu; Wang, Haibin; Liu, Xuemei. Phase stability in nanocrystalline partially ionic solids
08:50 [O53]	<u>Lee, Joonho</u> ; Sim, Kijoo. Prediction of the phase diagram of Sn-Ag nanoparticles
09:10 [O54]	<u>Gąsior, Władysław</u> ; Polański, Marek; Pstruś, Janusz; Dębski Adam. Studies on hydrogen storage materials from the Li-B and Ca-Li systems
09:30 [O55]	<u>Saengdeejing, Arkapol</u> ; Chen, Ying; Suzuki, Ken; Miura, Hideo; Matsuura, Masashi; Sugimoto, Satoshi. Electronic structures and formation mechanism of Nd-O in Nd-Fe-B magnets
09:50 [O56]	Kim, Na Rae; Shin, Kihyun; <u>Lee, Hyuck Mo</u> . Fabrication of Ag-Cu Nanoparticles Based on the Nano-Phase Diagram and Anti-Oxidation Effects
10:10 [O57]	<u>Wang, Fangfang</u> ; Xie, Ying; Chen, Jun; Fu, Honggang; Xing, Xianran. First-principles study on negative thermal expansion of PbTiO <sub>3</sub>
10:30	<b>Coffee break</b>

**Session 12 - CALPHAD Assessments & Experiments III**

<b>Chairs: Bo SUNDMAN / Gaowu QIN</b>	
10:50 [O58]	Hu, K.; <u>Gu, Z. F.</u> ; Cheng, G.; Rao, G.H.; Lin, R.S.; Hong, L.J. The isothermal section of the Nd-Mn-As phase diagram at 500 °C and 800 °C
11:10 [O59]	<u>Yin, Fucheng</u> ; Wang, Weilin; Zhao, Maoxiu; Li, Zhi; Wu, Yu. Experimental investigation and thermodynamic calculation of the Co-Si-Zn system
11:30 [O60]	<u>Rajagopal, Anand</u> ; 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 [O61]	Li, Shuai; Xie, Wei; Qiao, Zhiyu; <u>Cao, Zhanmin</u> . Critical evaluation and thermodynamic optimization of the V-O system
12:10 [O62]	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	<b>Lunch</b>

**Thursday (Afternoon), June 5<sup>th</sup>**

**Session 13 - Application of CALPHAD Method II**

<b>Chairs: Kiyohito ISHIDA / Zhenmin DU</b>	
13:50 [O63]	<u>Zhong, Yu</u> ; Yang, Mei; Chen, Ming. Application of computational thermodynamics in solid oxide fuel cell
14:10 [O64]	<u>Wang, Jianwei</u> ; Wang, Lijun; Wang, Ligen; Huang, Guojie; Cheng, Lei; Xiao, Wei. Application of CALPHAD method on the cracking control of Nb-containing bulk zirconium hydride
14:30 [O65]	<u>Li, Lin</u> ; Gao, Yi; He, Yanlin; Shi, Wen; Zhang, Mei; Lu, Xiaogang. Optimization of mechanical properties of high strength TRIP steels
14:50 [O66]	<u>Chizhko, Oleg</u> . Thermodynamic modeling of crystal structures for high-temperature anti-corrosion coatings
15:10 [O67]	<u>Brosh, Eli</u> . Modeling of the thermophysical properties of Fe-Ni alloys with application to calculation of high-pressure phase equilibria
15:30 [O68]	<u>Luo, Qun</u> ; 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
15:50	<b>Coffee break</b>

**Session 14 - CALPHAD Assessments & Experiments IV**

<b>Chairs: Hyuck Mo LEE / Xiaoyan SONG</b>	
16:10 [O69]	<u>Zhou, S.H.</u> ; Kramer, M.J.; Ott, R.T.; Napolitano, R.E. Energetic investigation of metastable Al <sub>60</sub> Sm <sub>11</sub> -ω, Al <sub>5</sub> Sm-π, Al <sub>4</sub> Sm-γ, Al <sub>1</sub> Sm <sub>3</sub> -α and Al <sub>4</sub> Sm-β phase formation
16:30 [O70]	<u>Roslyakova, Irina</u> ; Sundman, Bo; Dette, Holger. Modeling of thermo-physic properties for pure elements using segmented regression methodology
16:50 [O71]	<u>Broz, Pavel</u> ; Zelenka, Frantisek; Vřešťál, 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
17:10 [O72]	<u>Nuta, Ioana</u> ; Chatillon, Christian; Collas, Hervé; Artaud, Laurent; Guetta, Veronique; Heuer, Daniel. Vapor pressure measurements of LiF-ZrF <sub>4</sub> for Molten Salt Fast Reactor
17:30 [O73]	<u>Tang, Chengying</u> ; Shen, Wei; Xu, Wei; Wang, Jiang; Zhou, Huaiying. Size-dependent eutectic melting and thermodynamic properties of Ag-Cu alloy nanoparticles
17:50 [O74]	<u>Liu, Ya</u> ; Li, Daiyu; Su, Xuping; Wang, Jianhua. Microstructure differences and formation mechanisms of periodic-layered structure in Ni <sub>3</sub> Si/Zn system with Zn in vapor or liquid state
18:10	<b>Dinner</b>

**Thursday (Evening), June 5<sup>th</sup>**

**Software Demonstration Session**

<b>Chairs: Joonho LEE / Zhanmin CAO</b>	
19:30	<u>Chen, Qing</u> ; Kjellqvist, Lina. Thermo-Calc, DICTRA, and TC-PRISMA - A Continuing Integration
20:00	<u>Zhang, Fan</u> . PANDAT software for multi-component phase equilibrium calculation and precipitation simulation
20:30	Chartrand, Patrice; <u>Jung, In-Ho</u> . Recent development of FactSage software and database
21:00	<u>Effenberg, Günter</u> . MSI Eureka: Best practice for projects and CALPHAD
21:30	<u>Sundman, Bo</u> . Open Calphad Software



**Friday (Morning), June 6<sup>th</sup>**

**Session 15 - CALPHAD Assessments & Experiments V**

<b>Chairs: Tetsuo MOHRI / Sinn-wen CHEN</b>	
08:30 [O75]	<u>Chen, Shuanglin</u> ; Cao, Weisheng; Zhang, Fan; Zhang, Chuan; Zhu, Jun; Schmid-Fetzer, Rainer; Li, Qian; Zhang, Jieyu. Phase projection diagrams
08:50 [O76]	Zhao, Y.L.; Lu, Y.; Xu, W.W.; Jia, J.P.; Wang, C.P.; <u>Liu, X.J.</u> Steady-state dynamical phase diagram calculation of the U-Nb binary system under irradiation: ballistic effect
09:10 [O77]	<u>Kroupa, A.</u> ; Vrestal, J.; Boulet, Pascal; Dinsdale, A.; Watson, A.; Record, M.-Ch. The reassessment of the Al-Cu and Cu-Zn systems with respect to the $\gamma$ -brass phase
09:30 [O78]	<u>Chandra, Dhanesh</u> ; Mishra, Amrita; Shi, Renhai; Talekar, Anjali. Ternary phase diagram studies of Orientationally Disordered "Plastic Crystals"
09:50 [O79]	Ma, Ruting; <u>He, Wei</u> . The isothermal section of the phase diagram of Gd-Fe-Mn system at 773 K
10:10 [O80]	Hu, Renmin; He, Jin; Zhou, Han; Lu, Xionggang; <u>Li, Chonghe</u> . Thermodynamic modeling of Ti-Fe-Mn ternary system
10:30	<b>Coffee break</b>

**Session 16 - Microstructure Characterization & Simulation II**

<b>Chairs: George KAPTAY / Xingjun LIU</b>	
10:50 [O81]	<u>Shen, Jianyun</u> ; Zhao, Xushan; Feng, Xuankai ; Yuan, Gaihuan; Yue, Qiang. Study on formation mechanism of difference structures of ZrO <sub>2</sub> as Zr corrosion products
11:10 [O82]	Li, Guojian; Wang, Kai; Du, Jiaojiao; <u>Wang, Qiang</u> . Icosahedral-decahedral transformation in the Pd-Ag bimetallic cluster induced by Ag atomic segregation
11:30 [O83]	<u>Jian, Wei</u> ; Lai, Min; Ou, Xiaojian; Wu, Ruiwu; Wang, Hanbiao; Wang, Jiangyong. Mechanisms of metal-induced crystallization of amorphous silicon in Cu/a-Si and Ni/ a-Si bi-layered systems
11:50 [O84]	<u>Li, Mo</u> . Quantify grain growth from phase field modeling
12:10 [O85]	<u>Iikubo, Satoshi</u> ; Umebayasi, Tatsuki; Enoki, Masanori; Tokunaga, Tatsuya; Ohtani, Hiroshi. Thermodynamic properties in the Mg based alloy having long period stacking ordered structure
12:30	<b>Closing session</b>
13:00	<b>Lunch</b>

## List of Poster Presentations

- [P1] Jacob, Aurélie; Schmetterer, Clemens; Markus, Torsten; Singheiser, Lorenz; Gray-Weale, Angus. Thermodynamic description of Fe-W phase diagram using DFT and phonon calculations
- [P2] Wang, Zhengwei; Xu, Weiwei; Han, Jiajia; Wang, Cuiping; Liu, Xingjun. Investigation of half-metallic ferromagnetism in the Heusler compounds  $Sc_2VZ$  ( $Z=C, Si, Ge, Sn, Pb$ ) based on first-principles calculations
- [P3] Xu, Weiwei; Wang, Yi; Wang, Cuiping; Liu, Xingjun; Liu, Zi-Kui. Effects of doping Ta on the ideal strength of  $\gamma'$   $Co_3(Al, W)$  phase: A first principles study
- [P4] Zhang, Xi; Sluiter, Marcel HF. Ab initio prediction of vacancy properties in concentrated alloys: the case of fcc Cu-Ni
- [P5] Kong, Yi; Yang, Shunming; Pi, Jingwu; Chen, Li; Du, Yong. Coherent growth and its transformation to incoherent interface of CrAlN/TiN and CrAlN/ZrN nanomultilayers
- [P6] Wang, Jiong; Du, Yong; Shang, Shunli; Liu, Zi-Kui; Li, Yiwei. Effects of alloying elements on elastic properties of Al by first-principles calculations
- [P7] Wang, Jianchuan; Du, Yong; Sun, Lixian. Intrinsic defects in ammonia borane: density functional theory calculations augmented with van der Waals correction
- [P8] Gao, Qiannan; Shang, Shunli; Wang, Jiong; Wang, Jianchuan; Du, Yong; Liu, Zi-Kui. Effects of alloying elements on the stacking fault energies of dilute Al-based alloys
- [P9] Xin, Jinghua; Wang, Jianchuan; Du, Yong; Huang, Baiyun. The effect of subsurface vacancy on hydrogenation of Mg(0001) surface
- [P10] Wu, Shu-chang; Cheng, Ki-lin; Zhang, Chuan; Lin, Shih-kang. Ab initio-aided CALPHAD modeling for the Mo-Nb-Re ternary system
- [P11] Grabowski, B.; Korbmacher, D.; Glensk, A.; Duff, A.; Hickel, T.; Neugebauer, J. Ab initio description of dynamically unstable systems from zero Kelvin up to the melting point
- [P12] Zhou, Bi-Cheng; Shang, Shun-Li; Wang, Yi; Liu, Zi-Kui. Calculation of Dilute Tracer Diffusion Coefficients in Mg Using First-principles Methods
- [P13] Peng, Yingbiao; Zhang, Weibin; Du, Yong; Zhou, Peng; Chen, Weimin; Cheng, Kaiming; Zhang, Lijun; Liu, Shuhong; Wang, Shequan; Wen, Guanghua; Xie, Wen. Thermodynamic and diffusion databases of cemented carbides and their applications to development of new cemented carbides
- [P14] Wang, Jiang; Zhu, Chaofan; Fu, Gang; Cheng, Gang; Wang, Zhongmin; Rao, Guanghui; Zhou, Huaiying. Thermodynamic assessment of the Nd-Fe-B ternary system
- [P15] Zhu, Daiman; Li, Changrong; Guo, Cuiping; Du, Zhenmin. Thermodynamic assessment of the Ni-Sc binary system
- [P16] Liu, Lichang; Li, Changrong; Guo, Cuiping; Du, Zhenmin. Liquidus projection of the ternary Nb-Si-V system
- [P17] Wang, Jinsan; Li, Changrong; Guo, Cuiping; Du, Zhenmin. Thermodynamic Assessments of the Yb-Bi and the Yb-Te Systems
- [P18] Zhu, Jinjin; Lu, Yong; Liu, Xingjun; Wang, Cuiping. Experimental investigation and thermodynamic assessment of the Cu-Ni-Si ternary system
- [P19] Wang, Dong; Lu, Yong; Wang, Richu; Liu, Xingjun; Wang, Cuiping. Experimental investigation and thermodynamic calculation of phase equilibria in the Mg-Pb-Zn ternary system
- [P20] Antoni-Zdziobek, A.; Gospodinova, M.; Hodaj, F.; Bonnet, F.

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- Experimental investigation of the Fe-rich corner of the B-Fe-Ti system between 1373 K and 1723 K
- [P21] Yang, F.; Liu, H.S.; Cai, G.M.; Jin, Z.P.  
Experimental investigation of phase equilibrium in Al-Ti-Zr ternary system
- [P22] Kjellqvist, Lina.  
Thermodynamic assessment of the Cu-O-S System
- [P23] Li, Zhou; Mao, Huahai; Selleby, Malin.  
Re-assessment of the Co-Cr binary system
- [P24] Lindahl, Bonnie; Selleby, Malin.  
A thermodynamic assessment of the Al-Ti-V system
- [P25] Liu, Xuanton; Oikawa, Katsunari.  
Assessment of temperature and pressure dependence of molar volume and phase diagrams of Al, Cu, Si, and Zn
- [P26] Tong, Yonggang; Zhang, Hong; Bai, Shuxin; Ye, Yicong.  
Surface tension calculation of Si based and Zr based alloys in Si-Zr system
- [P27] Rzyman, Krzysztof; Maciąg, Tomasz; Kozubski, Rafał; Przeliorz, Roman.  
Determination of phase boundaries of Ni-rich corner of Ni-Al-Cr system by in situ experimental methods
- [P28] Kareva, Maria A; Kabanova, Elizaveta G; Kuznetsov, Viktor N.  
Revision of assessment of the Pd-Sn binary: replacing of polynomial description of liquid by association model
- [P29] Kim, Min-Su; Phan, Anh Thu; Lee, Hae-Geon; Kang, Youn-Bae.  
Phase Equilibria in the Fe-Mn-Al-C system: Experiment and Thermodynamic Modeling
- [P30] Moosavi-Khoonsari, Elmira.; Jung, In-Ho.  
A coupled experimental study and thermodynamic modeling of the Na<sub>2</sub>O-FeO-Fe<sub>2</sub>O<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> system
- [P31] Fima, Przemysław; Dębski, Adam.  
Li-Be and B-Be systems - experimental study
- [P32] Wu, Changjun; Liu, Ya; Su, Xuping; Peng, Haoping; Tu, Hao; Wang, Jianhua; Zhang, Yifan.  
Ternary compounds and phase equilibria in the Sn-Ni-V system
- [P33] Yang, Yang; Aune, Ragnhild E.  
Activity-Composition Relations and Thermodynamic Properties in Pt-V and Pt-Cr Alloys at 1500 °C
- [P34] Zhao, C.C.; Wang, C.P.; Lu, Y.; Li, T.; Liu, X.J..  
Observation of magnetically induced phase separation in the fcc phase and magnetic property in the Co-V system
- [P35] Xie, Di; Liu, Yuqin; Li, Zhiming.  
Phase equilibrium of the B-Cr-Nb system at the Cr-Nb side
- [P36] Dezso, Andras; Vasko, Gergely; Baumli, Peter; Kaptay, George.  
On the equilibrium Cu-content of the Sn-Ag-Cu liquid alloy with solid Cu
- [P37] Tang, Liwen; He, Huang; Zeng, Jianmin; Rao, Guanghui; Zhuang, Yinghong; Yan, Jialin.  
Phase equilibria in the Gd-Mn-Sn system at 450°C and magnetic property of compound Gd<sub>4</sub>Mn<sub>4</sub>Sn<sub>7</sub>
- [P38] Xu, Peng; Zhou, Kaiwen; Zhuo, Bingbing; Su, Xiaobo; Qin, Huagen; Zhuang, Yinghong; Yan, Jialin.  
Isothermal sections of the ternary Ge-Mn-Si and Mn-Si-Sn systems
- [P39] Yue, Qiang; Shen, Jianyun; Yuan, Gaihan; Zhao, Xushan; Yao, Meiyi; Peng, Jianchao; Zhang, Jinlong; Li, Geping.  
Experimental study on controversial precipitates in Fe-Nb-Zr system
- [P40] Shen, Jianyun; Chu, Maoyou; Feng, Xuankai; Chen, Yang.

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- CALPHAD study on Cu-rich clusters in RPV steel of nuclear power plant
- [P41] Guo, Cuiping; Li, Changrong; Du, Zhenmin.  
Thermodynamic modeling of the Pt–Te and Pt–Sb–Te systems
- [P42] Guo, Cuiping; Li, Changrong; Du, Zhenmin.  
Thermodynamic re-assessment of the Sb–Te system using the associate and ionic model for liquid phase
- [P43] Cui, Jiaxin; Guo, Cuiping; Li, Changrong; Du, Zhenmin.  
A thermodynamic assessment of the Se–Sn–Te system
- [P44] Cui, Jiaxin; Guo, Cuiping; Li, Changrong; Du, Zhenmin.  
A thermodynamic description of the Al–Ge–Ni system
- [P45] Ruan, J.J.; Wang, C.P.; Zhao, C.C.; Yang, S.Y.; Yang, T.; Liu, X.J.  
Phase equilibria of Co–Ti–V ternary system and the mechanical property of  $\gamma+\gamma'$
- [P46] Li, J.; Yang, S.Y.; Lu, Y.; Wang, C.P.; Liu, X.J.  
Experimental investigation and thermodynamic calculation of phase equilibria in the Nb–Si–Zr ternary system
- [P47] Jiang, H.X.; Wang, C.P.; Liu, X.J.  
Experimental determination of the phase equilibria in the Co–Mo–Cr and Co–Mo–Nb ternary systems
- [P48] Zhu, Jiahua; Yang, Shuiyuan; Xu, Weiwei; Wang, Cuiping; Liu, Xingjun.  
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