Oral presentations

Monday, June 12, 2017

08:45–09:00 Opening

Keynote lecture, chair: J.-C. Crivello

09:00–09:40 K1 Software tools for high-throughput CALPHAD from first-principles data

van de Walle Axel

Session: Configurational thermodynamics
Chairs: G. Kaptay - B. Sundman

09:40–09:55 O1 First Principles Calculation of the WS$_2$-WTe$_2$, Phase Diagram

Burton Benjamin

09:55–10:10 O2 Stability of NdFe$_{12}$(N) Series Compounds: A First-principles Study

Saengdeejeing Arkapol, Chen Ying

10:10–10:25 O3 Configurational thermodynamics of C in bcc Fe: a combined computational study

Yan Jiayi, Ruban Andrei

10:25–10:40 O4 Configurational energy of formation of alloys: Ising models vs the Cluster Expansion

Sanchez Juan

10:40–11:10 Coffee Break

Session: First principles and high-throughput
Chairs: A. Kroupa - B.-J. Lee


Arróyave Raymundo, Talapatra Anjana, Duong Thien, Son Woongrak, Prehn Evan, Gao Huihui, Radovic Miladin

11:25–11:40 O6 Comparison of calculated and experimental values of enthalpies of formation of intermetallic compounds.

Colinet Catherine, Tedenac Jean-Claude

11:40–11:55 O7 Nickel incorporation in Ti$_2$AlC ceramic

Lu Chengjie, Zhang Jie, Hug Gilles

11:55–12:10 O8 Ground state predictions for sulfide electrolytes

Iikubo Satoshi, Shimoyama Koichi, Kawano Shoya, Fujii Masafumi, Matsushita Masafumi, Shinmei Toru, Ohtani Hiroshi


Cui Yuwen, Guanglong Xu

12:25–14:00 Lunch
Session: Thermo-kinetics and diffusion
Chairs: J. Ågren - A. Costa e Silva

14:00-14:15 O10 Impacts of thermodynamic and kinetic model parameterisation on precipitation simulations - Case study of NbC precipitation in microalloyed steel
Povoden-Karadeniz Erwin, Kozeschnik E.

14:15-14:30 O11 Thermo-kinetic modeling for the growth/dissolution of α slabs and lamellae in Ti-55531 under continuous heating condition
Čen Fuwen, Xu Guanglong, Zhang Xiaoyong, Zhou Kechao

14:30-14:45 O12 Overcoming the Diffusion Bottleneck: Effect of Alloying Elements on Phase Transformations and Carbide Dissolution in Martensitic Stainless Steels
Miotti Bettanini Alvise, Delannay Laurent, Pardoen Thomas, Mithieux Jean-Denis, Badinier Guillaume, Pascal Jacques

14:45-15:00 O13 Temperature Dependence of Diffusivities from a Single Experiment - Experimental Technique and Evaluation Method
Engelhardt Hannes, Rettenmayr Markus

15:00-15:15 O14 Diffusivities and Atomic Mobilities in fcc Cu-Ni-Sn Alloys
Liu Yuling, Liu Dandan, Du Yong, Liu Shuhong

15:15-15:30 O15 Analytical model with interaction between species for growth and dissolution of precipitates
Gandin Charles-André, Guillemot Gildas

15:30-18:00 Poster session A, chair: M. Perrut

Session: Phase field and molecular dynamics
Chairs: A. Khvan - A. Gheribi

18:00-18:15 O16 Quantitative phase-field simulation of microstructure evolution in Ni-Al alloys during entire preparation process and its linking to mechanical property
Zhang Lijun, Cao Dongjia, Lin Yan

18:15-18:30 O17 Microstructure evolution during melting of single crystal superalloy: A combined experimental and computational study
Warnken Nik, Chen Xu, Slater Carl

18:30-18:45 O18 Matching time and spatial resolutions of rapid solidification: Dynamic TEM experiments coupled to CALPHAD-informed phase-field simulations
Perron Aurélien, Roehling John, Turchi Patrice, Fattebert Jean-Luc, McKown Joseph

18:45-19:00 O19 Glass Transition Temperature and Phase Diagrams of Butadiene Rubber and Styrene Butadiene Rubber: Molecular Dynamics Simulation
Lee Hyuck Mo, Ryu Myung Shin, Kim Hyoung Gyu, Bang K.

19:00-20:00 Free Time
20:00-21:00 Dinner
21:00-23:00 Evening session: Young Calphadian Meeting, chair: S. Gossé OR free poster viewing
- with the participation of C. Colinet, B. Sundman and B.-J. Lee
Tuesday, June 13, 2017

**Keynote lecture, chair: C. Guéneau**

09:00-09:40  **K2**  
Ab initio based multiscale modelling in physical metallurgy  
Willaime François, Lüthi B., Marinica M.C., Ventelon L., Rodney D.

### Session: First principles and nanos
**Chairs: P. Chartrand - S. Nishitani**

09:40-09:55  **O20**  
Phase stability and chemical composition of nanoprecipitates: A first principles study for the example of kappa carbides  
Hickel Tilmann, Dey Poulium, Dutta Biswanath, Friák Martin, Neugebauer Jörg

09:55-10:10  **O21**  
The size-dependent phase diagram for Ni-based systems by combination of CALPHAD and ab initio methods  
Kroupa Ales, Kana Tomas, Vykoukal Vit, Zemanova Adela, Svoboda Milan, Sob Mojmir, Pinkas Jiri

10:10-10:25  **O22**  
Constructing an As-Ga-In-Sn thermodynamic database for modelling the growth of InAs, GaAs and In$_x$Ga$_{1-x}$As nanostructures  
Ghasemi Masoomeh, Johansson Jonas

10:25-10:40  **O23**  
First-principles Calculation Assisted Thermodynamic Modeling of B-Ta and B-C-Ta System  
Xuemei Ouyang

10:40-11:10  Coffee Break

### Session: Interface and thin films
**Chairs: R. Arróyave - Y. Du**

11:10-11:25  **O24**  
Interface energy at limit radius in metallic system  
Nishitani Shigeto

11:25-11:40  **O25**  
Temperature and concentration dependent solid/liquid interfacial energies  
Lippmann Stephanie, Jung In-Ho, Palival Manas, Rettenmayr Markus

11:40-11:55  **O26**  
Modeling of metastable phase formation diagrams for sputtered thin films  
Chang Keke, Music Denis, To Baben Moritz, Lange Dennis, Bolvardi Hamid, Schneider Jochen

11:55-12:10  **O27**  
Calculation of phase diagrams with epitaxial orientations in Co-based binary alloy thin films  
Lu Yong

12:10-12:25  **O28**  
Thermodynamic study on grain boundary segregation  
Ohtani Hiroshi, Enoki Masanori, Higashide Yusuke

12:25-14:00  Lunch
**Session: Assessment: carbides and metallic systems**  
*Chairs: B. Lindhal - P. Turchi*

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<th>Time</th>
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<tr>
<td>14:00-14:15</td>
<td>O29</td>
<td>A new thermodynamic database of Ti(C,N)-based cermets and its application to the control of grain growth</td>
<td>Du Yong, Zhang Cong</td>
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<tr>
<td>14:15-14:30</td>
<td>O30</td>
<td>Thermodynamic assessment of the C-Zr system</td>
<td>Davey Theresa, Mellan Thomas, Fries Suzana, Finnis Michael</td>
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<tr>
<td>14:30-14:45</td>
<td>O31</td>
<td>From ternary experiments back to binary modeling: Li-Si-C example</td>
<td>Schmid-Fetzer Rainer, Liang Songmao, Drie Martin, Kozlov Artem, Rettenmayr Markus</td>
</tr>
<tr>
<td>14:45-15:00</td>
<td>O32</td>
<td>Modelling the Gibbs energy of Ag-Ni, Ag-Ge and Ag-Ge-Ni by calphad approach</td>
<td>Rajkumar V.B, Chen Sinn-Wen</td>
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<td>15:00-15:15</td>
<td>O33</td>
<td>Thermodynamic modelling of Long Periodic Stacking Ordered (LPSO) phases in Mg-Gd-Al ternary system</td>
<td>Kim Hongyeun, Ross Austin, Shang Shunli, Wang Yi, Kecskes Laszlo, Darling Kristopher, Liu Zi-Kui</td>
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<tr>
<td>15:15-15:30</td>
<td>O34</td>
<td>Phase equilibria of Pb-Sb-Se-Sn quaternary system</td>
<td>Chen Sinn-Wen, Chang Jui-Shen</td>
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<td>15:30-18:00</td>
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<td><strong>Poster session B, chair: M. Perrut</strong></td>
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**Session: Assessment: oxides**  
*Chairs: E. Povoden-Karadeniz - M. Selleby*

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<tr>
<td>18:00-18:15</td>
<td>O35</td>
<td>Phase relations in the ZrO$_2$-TiO$_2$-Al$_2$O$_3$ system: experimental study and thermodynamic assessment</td>
<td>Fabrichnaya Olga, Ilatovskaya Mariia, Savinykh G.</td>
</tr>
<tr>
<td>18:15-18:30</td>
<td>O36</td>
<td>Thermodynamic properties of oxide compounds estimated from polyhedron method</td>
<td>Jung In-Ho, Moosavi-Khoonsari Elmira, Wu Ting</td>
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<td>18:30-18:45</td>
<td>O37</td>
<td>Integrated experimental and thermodynamic modelling research on the multicomponent Pb-Cu-Fe-Zn-Ca-Si-O system</td>
<td>Shevchenko Maksym, Shishin Denis, Jak Evgueni</td>
</tr>
<tr>
<td>18:45-19:00</td>
<td>O38</td>
<td>Thermodynamic investigation of the Cr-O-U and Cr-O-Zr systems</td>
<td>Lindahl Bonnie, Alpettaz Thierry, Bonnailie Patrick, Brackx Emmanuelle, Chatain Sylvie, Domenger Renaud, Gossé Stéphane, Poissonnet Sylvie, Guéneau Christine</td>
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<td>19:00-20:00</td>
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<td><strong>Free Time</strong></td>
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<td>20:00-21:00</td>
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<td><strong>Dinner</strong></td>
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**Evening session: Computer session, chair: A. Pisch OR free poster viewing**

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<tr>
<td>21:00-21:30</td>
<td>C1</td>
<td>What is New in Thermo-Calc</td>
<td>Chen Qing</td>
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<tr>
<td>21:30-22:00</td>
<td>C2</td>
<td>Demonstration of Pandat software</td>
<td>Chen Shuanglin and Schmid-Fetzer Rainer</td>
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<tr>
<td>22:00-22:30</td>
<td>C3</td>
<td>Fact-Sage</td>
<td>Jung In-Ho</td>
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Wednesday, June 14, 2017

Keynote lecture, chair: I. Nuta
09:00-09:40 K3 Experimental Thermodynamics of Nuclear Materials
Konings R.J.M., Beneš O., Capelli E., Manara D., Popa K., Pavlov T., Vlahovic L.

Session: Experimental measurements I
Chairs: S. Lippman - B. Oudot
09:40-09:55 O39 Standard Enthalpies of Formation of Select Cu₂YZ Compounds
Nash Philip, Hasier John, Hawgood Mary, Kim George, Chen Wei
09:55-10:10 O40 Calorimetric determination of the formation enthalpy of ZnSb
Benigni Pierre, Berche Alexandre, Pothin Romain, Adenot Aurélien, Mikaelian Georges, Ayral Rose-Marie, Jund Philippe, Rogez Jacques
10:10-10:25 O41 Gaseous phase thermodynamics of organometallics: a TaN-precursor study
Nuta Ioana, Blanquet Elisabeth, Artaud Laurent, Collas Hervé, Chatillon Christian
10:25-10:40 O42 Thermodynamic Vaporization Studies of Lead Oxide and Sodium Oxide with Knudsen Effusion Mass Spectrometry
Kobertz Dietmar
10:40-11:10 Coffee Break

Session: Experimental measurements II
Chairs: P. Benigni - P. Nash
11:10-11:25 O43 A container-less electrochemical method to evaluate the thermodynamic properties of molten oxides and liquid alloys
Allanore Antoine, Nakanishi Bradley
11:25-11:40 O44 On the Quaternary System Ce-Ni-Zn-B
Roogl Peter, Failamani Fainan, Podloucky Raimund, Malik Zahida, Bursik Jiri, Grytsiv Andrij, Bauer Ernst
11:40-11:55 O45 Determination of phase equilibria in Fe-C-Mn-Al alloys for 3rd generation duplex steels
Mestrallet Aurore, Antoni-Zdziobek Annie, Emo Jonathan, Maugis Philippe, Hallstedt Bengt
11:55-12:10 O46 Alloy phase stability under electric currents
Lin Shih-Kang, Liu Yu-Chen
12:10-19:00 Excursion
19:00-20:00 Free Time
20:00-23:00 Conference Banquet
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<tr>
<td>09:00-09:40</td>
<td>Keynote lecture, chair: J.-M. Joubert</td>
<td>Thermodinamic and physical-property models for the production of primary aluminium</td>
<td>Chartrand Patrice, Gheribi Aimen Ernest, Wang K., Ouzilleau P., Robelin Christian</td>
</tr>
<tr>
<td>09:40-09:55</td>
<td>Session: Liquids and salts</td>
<td>Uncertainty quantification in ternary interpolation methods for thermodynamic properties of liquid alloys</td>
<td>Beyers Lesley, Van Den Bulck Amy, Wollants Patrick</td>
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<td>09:55-10:10</td>
<td>O47</td>
<td>Thermodynamic modeling and experimental investigations in the H$_2$O - HNO$_3$ - Sm(NO$_3$)$_3$ - Eu(NO$_3$)$_3$ - (C$_4$H$_9$O)$_3$PO system</td>
<td>Kovalenko Nikita, Maksimov Aleksey, Arkhipin Anatoly, Voronin Gennady</td>
</tr>
<tr>
<td>10:10-10:25</td>
<td>O48</td>
<td>Phosphoric acid and sodium phosphate: Extending the limit of aqueous electrolyte modelling</td>
<td>Wang Peiming</td>
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<td>10:25-10:40</td>
<td>O49</td>
<td>DFT/CALPHAD mixed method for the prediction of the thermal transport properties within aluminium electrolysis cells</td>
<td>Gheribi Aimen Ernest, Chartrand Patrice</td>
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<td>10:40-11:10</td>
<td>Coffee Break</td>
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<tr>
<td>11:10-11:25</td>
<td>Session: Assessment: metallic systems</td>
<td>Engineering applications of CALPHAD - some examples</td>
<td>Ågren John</td>
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<tr>
<td>11:25-11:40</td>
<td>O52</td>
<td>The formation of magnesiowustite in steelmaking slag evaluated experimentally and via computational thermodynamics</td>
<td>Costa e Silva Andre, Vieira Alan, Martins Antonio Augusto, Batista Rafaela, Avillez Roberto</td>
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<td>11:40-11:55</td>
<td>O53</td>
<td>Thermodynamic features of the Al-Mo and Al-Mo-Ti systems</td>
<td>Kriegel Mario, Klemm Volker, Fabrichnaya Olga, Freudenberger Jens, Leineweber Andreas</td>
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<td>11:55-12:10</td>
<td>O54</td>
<td>New assessment of the Al-Fe system</td>
<td>Zienert Tilo, Fabrichnaya Olga</td>
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<td>12:10-12:25</td>
<td>O55</td>
<td>A thermodynamic database for cast iron</td>
<td>Halstedt Bengt</td>
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<tr>
<td>12:25-14:00</td>
<td>Lunch</td>
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Session: 3rd generation and models
Chairs: C.-A. Gandin - B. Burton

14:40-14:55 O56 Experimental study and modeling of thermodynamic properties of the Ag-Cu system for the third generation of thermodynamic databases
Phiri Albina, Khvan Alexandra, Dinsdale Alan

14:55-15:10 O57 On the temperature dependence of excess Gibbs energy of solutions
Kaptyay George

15:10-15:25 O58 Modelling thermal vacancies within the CALPHAD approach
Liu Zi-Kui, Guan Pin-Wen

15:25-15:40 O59 Thermodynamic descriptions of pure Sn, Pb, Bi and Bi-Sn system from 0K using two state model for the liquid phase.
Khvan Alexandra, Dinsdale Alan, Phiri Albina

15:40-15:55 O60 About the limits of applicability of the Alkemade theorem for the construction of ternary liquidus surfaces
Stein Frank, He Cuiyun

15:55-16:10 O61 The Calphad Method - the Scientific use of Metastability
Sundman Bo

16:10-16:45 Coffee Break

Session: HEA and thermodynamic modelling
Chairs: N. David - R. Schmid-Fetzer

16:45-17:00 O62 Understanding Physical Metallurgy and Computational Design of High Entropy Alloys: Atomic Simulation and CALPHAD
Lee Byeong-Joo, Choi Won-Mi

17:00-17:15 O63 The fcc solid solution stability in multi-component system : towards high entropy alloys design
Bracq Guillaume, Laurent-Brocq Mathilde, Perrière Loïc, Pires Rémy, Crivello Jean-Claude, Joubert Jean-Marc, Guillot Ivan

17:15-17:30 O64 A Constraint Satisfaction Problem Approach to High-Entropy Alloy Design
Abu-Odeh Anas, Chaudhary Nayan, Gibbons Sean, Galvan Edgar, Kirk Tanner, Mao Hualai, Malak Richard, Arrógave Raymundo

17:30-17:45 O65 Phase stabilities of Ti materials with a focus on the thermodynamic modelling of metastable microstates
Marker Cassie, Shang Shunli, Zhao Ji-Cheng, Liu Zi-Kui

17:45-18:00 O66 Crystal structure relations among variants of the ω phase in titanium alloys and their modeling
Chen Hai-Lin

18:00-18:15 O67 Characterizing uncertainty of CALPHAD assessment, The Au-Pd case
Kuznetsov Victor

18:15-18:30 O68 Thermodynamic modelling of Cr-Fe-Nb-Sn-Zr system
Lafaye Paul, Crivello Jean-Claude, Toffolon-Masclet Caroline, Joubert Jean-Marc

18:30-18:45 O69 A New Approach of the CEF applied to the sigma phase modeling : Application to the thermodynamic re-assessment of the Nb-Al system using new experimental data.
Fiorani Jean-Marc, Araquito Pinto Da Silva Antonio Augusto, Carvalho Coelho Gilberto, Nunes Carlos, David Nicolas, Vilasi Michel

18:45-19:00 O70 Thermodynamic study on microstructure evolution during aging process in the Al-Cu binary alloy
Yabe Takahiro, Shibahara Shohei, Enoki Masanori, Ohtani Hiroshi

19:00-20:00 Free Time

20:00-21:00 Dinner
**Friday, June 16, 2017**

**Keynote lecture, chair: A. Antoni Zdziobek**

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<tr>
<td>09:00-09:40</td>
<td>K6</td>
<td><strong>Calphad Study of Planetary Condensation</strong></td>
<td>Saxena Surendra</td>
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**Session: Applications**

**Chairs: K. Frisk - F. Stein**

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<tr>
<td>09:40-09:55</td>
<td>O71</td>
<td>Phase diagrams of alloys under pressure</td>
<td>Makov Guy, Emuna Moran, Yahel Eyal, Greenberg Yaron</td>
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<td>09:55-10:10</td>
<td>O72</td>
<td>Thermodynamic description of the lithium manganese oxide as cathode materials for lithium-ion batteries</td>
<td>Zhang Weibin, Cupid Damian, Seifert Hans</td>
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<td>10:25-10:40</td>
<td>O74</td>
<td>A CALPHAD approach to modelling of slag viscosities</td>
<td>Hack Klaus, Yakshenshikh Elena, Wu Guixuan, Mueller Michael, Jantzen Tatjana</td>
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<td>10:40-11:10</td>
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<td><strong>Coffee Break</strong></td>
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**Session: Nuclear materials, catalysts and cemented carbides**

**Chairs: S. Gossé - A. Perron**

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<td>11:25-11:40</td>
<td>O76</td>
<td>CALPHAD approach: a complementary way to determine the corrosion pathway of PuAl alloys stabilized in delta-phase</td>
<td>Oudot Benoit, Ravat Brice, Jolly Lionel, Perron Aurélien, Turchi Patrice, Guéneau Christine, Delaunay François</td>
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<tr>
<td>11:40-11:55</td>
<td>O77</td>
<td>PdZn Intermetallic compound: A pseudoelement of Cu for catalysis</td>
<td>Tsai An Pang, Kameoka Satoshi, Shimoda Masahiko, Ishii Yasushi</td>
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<tr>
<td>11:55-12:10</td>
<td>O78</td>
<td>Design of grain growth inhibitors and analysis of mechanical properties in ultra-fine WC-10Co cemented carbides based on thermodynamic calculations</td>
<td>Haixia Tian, Peng Yingbiao, Du Yong</td>
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<td>12:25-12:40</td>
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<td><strong>Closing</strong></td>
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<td>12:40-14:00</td>
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<td><strong>Lunch</strong></td>
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