

# **28<sup>th</sup> Annual MSIT Meeting**

## **International Seminar on Heterogeneous Multicomponent Equilibria**

09 – 14 March 2014, Schloss Ringberg, Tegernsee, Germany

*Organized by*

*MSI, Materials Science International Services GmbH, Stuttgart  
Max-Planck-Institute for Solid State Physics, Stuttgart  
Max-Planck-Institute for Chemical Physics of Solids, Dresden*

# A G E N D A

## SUNDAY, March 9, 2014

Starting 15:00		ARRIVAL
16:09	Tegernsee train station	Shuttle 1 to the castle
17:09	Tegernsee train station	Shuttle 2 to the castle
19:00	Gartenzimmer	Get Together (snack bar)

## MONDAY, March 10, 2014

### Day of Science: Fundamentals of Materials Chemistry. Dedicated to Fred Hayes

9:00	Konferenzraum	Chair: Günter Effenberg	Opening by <b>Günter Effenberg (MSI, DE)</b> . "Scope of the 28 <sup>th</sup> MSIT Meeting"
9:15			<b>Andy Watson (University Leeds, UK)</b> Materials chemistry introduction, the Fred Hayes Memorial Day
9:45			<b>Rainer Schmid-Fetzer (TU Clausthal, DE)</b> Phase Diagrams: Primer, Applications and Traps
10:30	Konferenzgebäude		Coffee
11:00	Konferenzraum	Chair: Günter Effenberg	<b>Peter Franz Rogl (University Vienna, AT)</b> Applied crystallography
11:30			<b>Torsten Markus (Forschungszentrum Jülich, DE)</b> Experimental methods (thermal experiments, mass spectrometry)
12:00			<b>Alexandra Khvan (National University of Science and Technology "MISIS", RU)</b> <b>Andy Watson (University Leeds, UK)</b> Experimental methods (caloric, others)
12:30	Speisesaal		Lunch
14:00	Konferenzraum	Chair: Andy Watson	<b>Carlos Ziebert (KIT, Karlsruhe, DE)</b> Electrochemical-calorimetric studies for the determination of heat data of lithium-ion cells
14:30			<b>Alan Dinsdale (National University of Science and Technology "MISIS", RU)</b> Calculation of phase equilibria from critically assessed thermodynamic data
15:00			<b>Erich Wimmer (Materials Design Inc., Montrouge, FR)</b> Fundamentals of "Ab initio" calculations

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15:30	Konferenz- gebäude	Coffee
16:00	Konferenzraum  Chair: Andy Watson	<b>Catherine Colinet (INP CNRS, Grenoble, FR) and Jean-Claude Tedenac (Univ. Montpellier, FR)</b> Applied "Ab initio" calculations
16:30		<b>Nils Warnken (University of Birmingham, UK)</b> Morphology (experimental studies and fundamentals of computer aided methods)
17:00		<b>Olga Fabrichnaya (TU Bergakademie, Freiberg, DE)</b> Phase diagram in ZrO <sub>2</sub> - based system and thermodynamic description for modelling ceramic component of TRIP matrix composite
17:20		<b>Tilo Zienert (TU Bergakademie, Freiberg, DE)</b> Experimental investigations in the Al-Fe-Si systems
17:40		<b>Günter Effenberg, (MSI, Stuttgart, DE)</b> MSI Eureka
18:10		<b>Ales Kroupa (Institute of Physics of Materials, Brno, CZ)</b> TOFA announcement
18:15		<b>Günter Effenberg, (MSI, Stuttgart, DE)</b> Summary Day of Science
18:30	Speisesaal	Dinner (Bavarian Buffet)

# A G E N D A

**TUESDAY, March 11, 2014**

8:00 – 9:00	Speisesaal	Breakfast	
9:00	Konferenzraum	Chair: Peter Rogl	<b>Lesley Chown (University of the WITS, SA)</b> Introduction of the new participant
9:10			<b>Gerda Rogl (Universität Wien, Vienna, AT)</b> Introduction of the new participant
9:20			<b>Mikael Perrut (ONERA, Châtillon, FR)</b> Introduction of the new participant
9:30			<b>Hsien Ming Hsiao (Technische Universität Clausthal, Clausthal, DE)</b> Introduction of the new participant
9:40			<b>Cong Zhang (Central South University, Changsha, CH)</b> Introduction of the new participant
9:50			<b>Svitlana Iljenko (MSI, Stuttgart, DE)</b> Working Structure of Groupwork
10:00			<b>Arno Lehmann (MSI, Stuttgart, DE)</b> MSI Collaboration Tool
10:10			<b>Oleksandr Dovbenko (MSI, Stuttgart, DE)</b> MSI Graphics Editor
10:20			Konferenzgebäude
<b>DFG SPP 1473</b>			
10:50	Konferenzraum	Chair: Rainer Schmid Fetzner	<b>Arno Lehmann (MSI, Stuttgart, DE)</b> Recent enhancements of LIBworks
11:05			<b>Maren Lepple (KIT, Karlsruhe, DE)</b> Thermodynamic Investigations and Modeling of Copper and Iron Oxides Used as Conversion Electrodes in Lithium Ion Batteries
11:20			<b>Nicolas Mayer (KIT, Karlsruhe, DE)</b> Li-Cu-Co-O Conversion Type Anodes for Lithium Ion Batteries
11:30			<b>Keke Chang (RWTH, Aachen, DE)</b> Theoretical study of cathodes in lithium ion batteries
11:45			<b>Dajian Li (KIT, Karlsruhe, DE)</b> presentation of recent work on Li Ion Batteries
12:00			<b>Siaufung Dang (FZ Jülich, DE)</b> Ab Initio Coupled Thermodynamic Modelling of Cathode Materials for Li-Ion Batteries
12:15			<b>Elke Schuster (KIT, Karlsruhe, DE)</b> Electrochemical-Calorimetric Studies on Lithium Ion Pouch Cells
			Group-Work  Critical Evaluation and Review of Materials Systems <i>(allocated group rooms)</i>

# AGENDA

12:30	Speisesaal	Lunch	
14:00	Konferenzraum Chair: Rainer Schmid-Fetzer	<b>Marc Strafela (KIT, Karlsruhe, DE)</b> <i>Thin Film Cathodes for Lithium Ion Batteries in the Material System Li-Ni-Mn-Co-O.</i>	Group-Work continued (allocated group rooms)
14:15		<b>Jian Peng (KIT, Karlsruhe, DE)</b> Thermodynamics and Microstructure Development in Alloys of Ni-Al-Cr-Mo System	
14:30		<b>Felix Rieger (KIT, Karlsruhe, DE)</b> Thermodynamic Modelling and Experimental Investigation of the System Fe-Cr-Y-O.	
14:45	allocated group rooms	<u>Group-Work</u> <i>Critical Evaluation and Review of Materials Systems</i>	
15:30	Gartenzimmer	Coffee	
16:00	allocated group rooms	Group-Work continued (allocated group rooms)	
18:30	Speisesaal	Dinner	
21:00	Speisesaal	Feuerzangenbowle	

## WEDNESDAY, March 12, 2014

8:00 – 9:00	Speisesaal	Breakfast	
9:00	allocated group rooms	<u>Group-Work</u> Critical Evaluation and Review of Materials Systems	
10:30	Gartenzimmer	Coffee	
11:00	allocated group rooms	Group-Work continued	
12:30	Speisesaal	Lunch	
14:00	allocated group rooms	Group-Work continued	
15:30	Gartenzimmer	Coffee	
16:00	allocated group rooms	Group-Work continued	
18:30	Speisesaal	Dinner	
20:00	Konferenzraum Chair: Günter Effenberg	Discussion of evaluation problems found at groupwork	

# A G E N D A

## THURSDAY, March 13, 2014

8:00 – 9:00	Speisesaal	<i>Breakfast</i>	
9:00	allocated group rooms	<u>Group-Work</u> Critical Evaluation and Review of Materials Systems	
10:30	Gartenzimmer	<i>Coffee</i>	
11:10	allocated group rooms	Group-Work continued	
12:30	Speisesaal	<i>Lunch</i>	
13:30	Gate of the castle	Walking (weather dependent and optional)	Group-Work continued (allocated group rooms)
15:30	Gartenzimmer	<i>Coffee</i>	
16:00	allocated group rooms	Group-Work continued	
18:30	Speisesaal	<i>Dinner</i>	
20:00	Konferenzraum Chair: Günter Effenberg	<b>Discussion of evaluation problems found at groupwork</b>	

## FRIDAY, March 14, 2014

8:00 – 9:00	Speisesaal	<i>Breakfast</i>	
9:00	allocated group rooms	<u>Group-Work</u> Critical Evaluation and Review of Materials Systems Group-Work continued	
10:30	Gartenzimmer	<i>Coffee</i>	
11:00	allocated group rooms	<u>Group-Work</u> Critical Evaluation and Review of Materials Systems Group-Work continued	
10:30	Gartenzimmer	<i>Coffee</i>	
11:00	Konferenzraum Chair:	<u>Group-Work</u> Critical Evaluation and Review of Materials Systems Group-Work continued	
12:00	Speisesaal	<i>Lunch</i>	
till 14:00		Departure Please note: MSI will <b>not</b> give a shuttle service to the station	
		Evaluation work to be completed remotely till 15.06.2014	