



**Materials with New Design for Improved Lithium Ion Batteries,
Werkstoffe mit neuem Design für verbesserte Lithium-Ionen-Batterien**

**Final Colloquium Priority Programme 1473
German Research Foundation**

Homepage WeNDeLIB: www.spp1473.kit.edu

Event days: November 23 - 25, 2016
Location: FTU – AULA (Fortbildungszentrum für Technik und Umwelt)
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Wednesday; November 23, 2016

19:00 Get-together, Dinner
(BADISCH BRAUHAUS, Stephanienstr. 38-40, 76133 Karlsruhe)

Thursday; November 24, 2016

9:00 – 9:10 *O. Kraft (Vice President of KIT): Welcome Address*
9:10 – 9:25 *H.J. Seifert: Coordination - Priority Programme WeNDeLIB*
9:25 – 10:25 **JP 8:** Nanocomposites as anode materials for lithium ion batteries: synthesis, thermodynamic characterization and modeling of nanoparticulate silicon dispersed in SiCN(O) and SiCO-based matrices
9:25 – 9:45 **JP 8.2** *M. Graczyk-Zajac:* Novel Si/Sn-containing SiOC/SiCN nanocomposites: toward electrochemically stable lithium storage in silicon/tin
9:45 – 10:05 **JP 8.3** *D. Cupid:* Thermodynamic characterization of novel SiOC materials for lithium storage
10:05 – 10:25 **JP 8.1** *J. Rohrer:* Si and SiOC as anode materials for Li-ion batteries: insights from atomistic modelling

Coffee break (30 min)

10:55 – 11:55 **JP 4:** Experimental thermodynamics and phase relations of new electrode materials for lithium ion batteries
10:55 – 11:15 **JP 4.1** *D. Li:* Thermodynamic modeling and simulation of intermetallic material systems for lithium ion batteries
11:15 – 11:35 **JP 4.2** *A. Beutl:* Phase diagrams, structures and thermochemistry in Cu-Li-Sn, Cu-Sb-Sn and constituent binaries
11:35 – 11:55 **JP 4.3** *H. Giel:* Thermodynamic data determination by KEMS, CT, and coin cell calorimetry (CCC)
11:55 – 12:15 **JP 6:** Linking of model and commercial active materials for lithium ion batteries by in-situ determination of thermodynamic and kinetic data
11:55 – 12:15 **JP 6.2** *H. Wulfmeier, A. Omelcenko:*
High-Temperature Thin-Film Calorimetry

Lunch (60 min)

- 13:15 – 14:15** **JP 3:** Design of an all solid state thin film lithium ion battery and their electrochemical-thermodynamic modeling and evaluation
- 13:15 – 13:35** **JP 3.1** *K. Chang:* Quantum mechanically guided design of amorphous Si–Al–M (M = 3d metals) anodes for Li ion batteries
- 13:35 – 13:55** **JP 3.2** *M. Masoumi:* Thermochemistry and phase stabilities of NMC-based cathode materials with selected compositions
- 13:55 – 14:15** **JP 3.3** (funded during 1st period) *S. Ulrich:* Development of cathode materials for lithium ion batteries based on thin film technology
- 14:15 – 14:55** **JP 9:** Phase stability of alloy-type lithium storage anode materials
- 14:15 – 14:35** **JP 9.1** *M. Drüe:* Phase stability of alloy-type lithium storage anode materials: production and characterization of Li-C+x alloys
- 14:35 – 14:55** **JP 9.2** *S. Liang:* Phase stability of alloy-type lithium storage anode materials: Thermodynamics and phase equilibria of the Li-Si-Sn-C alloy system
- Coffee break (30 min)**
- 15:25 – 16:05** **JP 10:** Rational tuning and thermodynamic characterization of lithium silicides and lithium iron phosphate as electrode materials for lithium ion batteries – nano-scaling guided by calorimetric, thermokinetic and theoretical investigations
- 15:25 – 15:45** **JP 10.2** *F. Biedermann:* Calorimetric and hydrogen sorption investigations for the thermodynamic characterization of the Li-Si-System
- 15:45 – 16:05** **JP 10.3** *S. Schwalbe:* Computational thermodynamics applied to lithium silicide battery materials
- 16:05 – 16:35** ***D. Cupid:* Focus Group Calorimetry**
- 16:35 – 16:55** **JP 11.1** (funded during 1st period) *T. Hammerschmidt:* Spatially resolved modeling and characterization of (de-)intercalation in Li-ion battery materials
- 16:55 – 17:15** **JP 14.2** (funded during 1st period) *H. Schmidt:* Lithiation of amorphous silicon electrodes in Li-ion batteries: investigations with Neutron Reflectometry and Secondary Ion Mass Spectrometry
- 17:15 – 17:35** **JP 13.2** (funded during 1st period) *G. Schmitz:* Phase separation and intercalation kinetics in LiFePO₄ thin film battery electrodes
- 17:35 - 18:45** **Poster Session (finger-food served)**
- Friday; November 25, 2016**
- 09:15 – 10:35** **JP 12:** Thermodynamics and kinetics for stabilization of conversion-type electrodes for LIB based on nano 3d transition metal oxide composites
- 09:15 – 09:35** **JP 12.1** *G. Balachandran:* Electrochemical performance and mechanism of 3d-transition metal ferrites MFe_2O_4 (M = Fe, Co, Ni, Cu, Sn) as conversion type model systems for Li-Ion batteries
- 09:35 – 09:55** **JP 12.2** *R. Adam:* Microstructural consequences of the coexistence of conversion and intercalation mechanisms in conversion reaction based lithium ion batteries
- 09:55 – 10:15** **JP 12.3** *N. Mayer:* Correlation between thermochemistry and electrochemistry for the conversion mechanism in transition metal oxide based anode materials
- 10:15 – 10:35** **JP 12.4** *Y. Qian:* The effect of film-forming additives in improving the electrochemical performance of NMC/CuO lithium ion batteries
- 10:35 – 10:55** **JP 10.1 (funded during 1st period)** *H. Emmerich:* Towards a more accurate phase-field description of depletion zones and nanoscale kinetics in Li-ion battery materials
- 11:00** **H.J. Seifert: Final Remarks**