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](http://www.spp1473.kit.edu)

**Event days:** November 23 - 25, 2016
**Location:**
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Hermann-von-Helmholtz-Platz 1
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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

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
13:55 – 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 – 14:35  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
10:35 – 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