Thermodynamic Assessments of Systems Evaluated in the WENDELIB Priority Program for Li-Ion Batteries

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ABSTRACT

The priority program "*Materials with New Design for Improved Lithium Ion Batteries (WeNDeLIB)*" funded by the German Research Foundation has been instituted to promote scientific research on the relationships between thermodynamics, kinetics, crystal chemistry and micro-/nanostructures of new materials for lithium ion batteries.

This scientific program recognizes that materials thermodynamics play a key role in the development of electrode materials with improved performance characteristics. Several candidate materials systems have been investigated and key experiments have been combined with the thermodynamic modelling to produce self-consistent thermodynamic descriptions which reproduce the measured thermochemical, phase diagram, and electrochemical data.

Particularly, intermetallic and oxide systems have been considered as new electrode materials with largely improved capacities exhibiting either the intercalation or conversion mechanism for lithium storage.

In this work, the thermodynamic modelling and assessments of the Cu-Sn and Li-Sn intermetallic systems and of the Li-Mn-O and Li-Cu-O oxide systems will be presented. The measurement of key thermochemical data in the metallic and oxide systems will be emphasized, and the ability of the assessed descriptions to calculate coulometric titration curves will be highlighted.