Thermochemical Investigations, Data Determination, and FactSage Calculations for Li-Ion Batteries

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ABSTRACT

Li-Ion batteries are well recognized as a possible and efficient way to store electric energy. For use in mobile applications, however, these batteries have to meet several design criteria, such as the number of charge/discharge cycles, energy density and safety. The latter is one of the crucial requirements that has so far prevented the wide spread use of these batteries.

Computational Thermodynamics is an essential tool for the further development of such devices. Thus, the availability of a comprehensive database of thermodynamic key values will allow further predictive modeling of the functionality of Li-ion batteries on one hand but also on the long term performance and degradation effects on the other hand.

This includes the kinetics of the Li-intercalation and de-intercalation and the relevant improvement towards higher operation times. However, the knowledge of basic thermodynamic data concerning the battery relevant systems is very weak.

The presentation will focus on the basics of the methods as well as on the determination of thermodynamic key data for Li ion battery systems as well as on the potential of computer based modeling for further understanding of battery relevant reactions.