Thermodynamic modeling of copper and iron oxides used as conversion electrodes in lithium ion batteries

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Compounds in binary and ternary sub-systems of the Li-Cu-Fe-O system are promising electrode materials for lithium ion batteries which exhibit the conversion mechanism. Thermodynamic descriptions of the multi-component systems can be used to predict equilibrium open circuit voltages and plateau capacities. Experimentally determined thermochemical and thermodynamic data are key input data for the thermodynamic optimization. For the experimental investigations, samples were prepared using the mixed oxide and sol-gel self combustion methods and were characterized using XRD and ICP-OES. Enthalpies of formation of different compounds were determined using high temperature oxide drop solution calorimetry in molten 3Na2O.4MoO3 solvent at 700 °C. The phase stabilities were measured in argon and argon/oxygen mixtures using simultaneous thermal analysis. Additionally, the heat capacities of the materials were measured using differential scanning calorimetery. This data and evaluated literature values were used to obtain a consistent thermodynamic description of the sub-systems Li-Cu-O and Li-Fe-O. Subsequently, coulometric titration curves of different starting compounds were calculated, which give the open circuit voltage along a selected composition path.