Thermodynamic dataset of electrode materials in lithium ion batteries

Keke Chang

Materials Chemistry, RWTH Aachen University, Aachen
E-mail address: chang@mch.rwth-aachen.de

$LiCoO_2$, $LiNiO_2$ and $Li(Co,Ni)O_2$ have been studied as electrode materials in lithium ion batteries. The corresponding systems, O3 and O2 structural $LiCoO_2$–CoO_2, O3 structural $LiNiO_2$–NiO_2 and $Li(Co,Ni)O_2$–$(Co,Ni)O_2$ were investigated using the CALPHAD approach. All the phases are described with appropriate sublattice models and parameters. The calculations on their phase diagrams and thermodynamic properties are in good agreement with literature data and the obtained *ab initio* results. Using the thermodynamic description derived in this dissertation, the cell voltages of Li/$LiCoO_2$ and Li/O3-$Li(Co,Ni)O_2$ are well reproduced.