

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Control of thermodynamics and kinetics through anion substitution in metal borohydrides YOUNG-SU LEE, YOONYOUNG KIM, JAE-HYEOK SHIM, YOUNG WHAN CHO, Korea Institute of Science and Technology, Republic of Korea — High thermal stability of metal borohydrides is one of the bottlenecks in adopting them for practical hydrogen storage materials. For this reason, much effort has been put toward lowering their thermal stability. One of the common routes taken to achieve this aim is to mix with other borohydrides or alanes of less thermal stability hoping to make a compound or an alloy of intermediate stability. Recent studies have proposed a possibility where F^- or Cl^- anions could incorporate into the lattice of alanes or borohydrides replacing H^- or BH_4^- anions, thus modifying the thermal stability of these materials. We present here a combined experimental and theoretical study on the anion substitution in $Ca(BH_4)_2$ and $LiBH_4$. Both thermodynamic and kinetic aspect will be discussed.

Young-Su Lee
Korea Institute of Science and Technology, Republic of Korea

Date submitted: 30 Nov 2008

Electronic form version 1.4