Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Dehydrogenation of $LiBH_4$ nanoclusters: A first-principles study
EBRAHIM HAZRATI, FILIPE VASCONCELOS, ESM, IMM, Radboud University, GEERT BROCKS, CMS, University of Twente, ROBERT DE GROOT, GILLES DE WIJS, ESM, IMM, Radboud University — Recent experimental studies[1,2] show faster desorption kinetics, improved reversibility and more favorable thermodynamics for confined $LiBH_4$ nanoparticles than the bulk. Using density functional theory calculations, we first discuss the geometries and energetics of $LiBH_4$, LiH, LiB, Li and B clusters. Secondly, we study the effects of particle size on the decomposition pathway of $LiBH_4$ clusters. Our calculations show that only very small clusters of $LiBH_4$ (up to 12 formula units) are significantly destabilized relative to the bulk. High stability of small clusters of $LiBH_4$ originates from the fact that surface energies are very low for bulk $LiBH_4$. (100), (010), (101) and (011) surfaces are almost degenerate with surface energies of 0.113, 0.102, 0.115 and 0.097 J/m^2, respectively. Clusters of LiH, LiB, Li and B are more strongly destabilized than the $LiBH_4$ clusters upon decreasing the cluster size. We show that, in contrast to the bulk, destabilized clusters of $LiBH_4$ decompose to $(LiB)_n$ clusters. Finally, we present some of our preliminary NMR chemical shift results for different $LiBH_4$ surface terminations.

[1]A.F. Gross et al. J. Phys. Chem. C 112, 5651, 2008
[2]X. Liu et al. Chem. Mater. 23, 1331, 2011

Gilles de Wijs
ESM, IMM, Radboud University

Date submitted: 22 Dec 2011 Electronic form version 1.4