A NOVEL AMMINE LITHIUM ALUMINUM BOROHYDRIDE MATERIAL FOR HYDROGEN STORAGE

Huynh-Duc NGUYEN[a], Parviz HAJIYEV[a], Umit B. DEMIRCI[b], Gérard GEBEL[a]

[a] Univ Grenoble Alpes, CEA, Liten, DTNM, 38000 Grenoble, France

[b] Institut Européen des Membranes, IEM – UMR 5635, ENSCM, CNRS, Univ Montpellier, Montpellier, France

E-mail: huynh-duc.nguyen@cea.fr

A novel solid ammine lithium aluminum borohydride $LiAl(BH_4)_4(NH_3)_6$ compound has the potential to be a good hydrogen storage material with 17.3 wt.% theoretical hydrogen capacity. It is synthesized at room temperature from $LiAlH_4$ and $(CH_3)_2S\text{-}BH_3$ precursors using the solvothermal method in liquid ammonia, which is a one-pot synthesis method that produces no solid byproducts or does not require the synthesis of pyrophoric compounds like $Al(BH_4)_3$.

X-ray powder diffraction analysis shows that the structure of $LiAl(BH_4)_4(NH_3)_6$, which has yet to be reported in the literature, does neither fit with known compounds such as $Li_2Al(BH_4)_5(NH_3)_6$[1] nor $Al(BH_4)_3(NH_3)_6$[2]. Hence, the Rietveld refinement is performed to resolve the crystalline structure of this compound. Furthermore, FTIR, Raman, and MAS NMR spectroscopy are used to fully characterize $LiAl(BH_4)_4(NH_3)_6$. FTIR and Raman spectra reveal the presence of $[BH_4]^-$ and NH_3 groups, and the valence vibration of the Al-N bond in the coordination octahedron $[Al(NH_3)_6]^{3+}$. These findings are also supported by the ^{11}B and ^{27}Al MAS NMR spectra.

The dehydrogenation properties are investigated using TGA/DSC/MS/PCT characterization tools. The results show that this material decomposes exothermically at 154°C, releasing 12.5 wt.% H_2 with a purity of 96 mol% while the main contaminant being NH_3. The hydrogen purity is improved to >99.0 mol% using the isothermal pretreatment method. In addition, using the Kissinger equation for kinetic analysis of dehydrogenation process, the activation energy is found to be 143.1 kJ/mol, which is comparable to similar compound such as ammonia borane[3].

On another note, the amorphous Li-Al-B-N-H dehydrogenation product is unable to be rehydrogenated directly. This necessitates chemical regeneration. Hence, *in situ* XPS is being utilized to better understand the chemical composition and develop better chemical regeneration roots, much like its simpler synthesis process.

References

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Picture of Author	Short Biography of Author
	Huynh-Duc Nguyen is a PhD student at The French Alternative Energies and Atomic Energy Commission (CEA) since November 2020. He works on the hydrogen storage materials and their regeneration. Huynh-Duc earned a degree in process engineering and a master's degree in chemistry, specialty of processes for valorization of renewable resources from the University of Technology of Compiègne (France), graduating in 2019. He currently lives in Grenoble.