4th International Symposium on
Energy Challenges & Mechanics
- working on small scales

11-13 August 2015
Aberdeen, Scotland, UK

Ammonia borane and its amine-borane derivatives for hydrogen production. What about homogeneous catalytic dehydrogenation?

Emilia Sicilia[1*], Valeria Butera[1], Ida Ritacco[1] and Nino Russo[1]

[1] *Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Ponte P. Bucci, 87036 Arcavacata di Rende (CS)*

Accepted for publication on 3rd March 2015

In recent years, amine-borane adducts, particularly parent ammonia-borane, $H_3N{-}BH_3$ (AB), have attracted great interest as H_2-vectors for chemical hydrogen storage, most recently revived by reports on the regeneration of spent fuels. Aside from energy storage applications, amine-boranes dehydrogenation/dehydrocoupling is also highly attractive for the synthesis of polymeric B−N-materials. Although the combination of hydridic B–H and protic N–H bonds within the AB and amine-borane molecules mean that they are susceptible to thermally induced hydrogen release, the temperatures at which this occurs are impractically high (110–200 ◦C). This factor has, in turn, resulted in a focus upon the use of catalytic methods to cause hydrogen evolution and concomitant B–N bond formation for the AB molecule itself, and for a wide variety of di- and mono-alkylamine borane molecules. Experimental and theoretical investigations carried out so far have shown that metal-mediated dehydrocoupling reactions of amine-boranes are very complex processes and both the mechanism and the final outcome depend on the nature of the catalyst in terms of identity of the metal centre, ligands and bonding modes. The nature of the amine-borane alkyl groups also influences the course of the process. However, what is lacking in this burgeoning field is a unified model in which new mechanistic clues can be put in context. We report here the outcomes of the DFT theoretical investigation of metal catalyzed dehydrogenation and dehydrocoupling reactions of amine-boranes as potential hydrogen storage materials. All the presented results show how theoretical investigations should be helpful in disentangling the experimentally envisaged mechanistic details and providing precious hints for the improvement of existing catalysts.

Keywords: amine-boranes, dehydrogenation, homogeneous catalysts, DFT