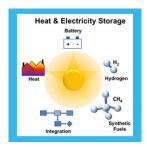
## **Annual Symposium 2014**



Contribution ID: 30 Type: not specified

## CATALYZED H SORPTION MECHANISM IN ALANATES

Tuesday 4 November 2014 12:00 (1h 15m)

Bogdanovic [1] presented the Ti-catalyzed hydrogen sorption in NaAlH4. The mechanism of the catalysis remains unclear despite the large number of proposed models. We presented a completely symmetric mechanism where the catalyst had a well-defined function. Firstly, we focused exclusively on understanding the main intermediate steps in the dehydrogenation and rehydrogenation of MAlH4 and M3AlH6 (where M= Li, Na, and K) based on thermodynamic considerations. In this manner, the Gibbs free energy values of each possible step were calculated based on experimental determined thermodynamic data (enthalpies and entropies) of individual hydrides, MAlH4, M3AlH6, and MH. Secondly, the values for the activation energies, based on the intermediates MH and AlH3 were obtained. Lastly, we presented an atomistic model, where the catalyst acted as a bridge to transfer the M+ and H- from AlH4- to AlH63- and finally to form MH based on thermodynamic considerations. The proposed mechanism is symmetric and the catalyst is active on the intermediates NaH and AlH3 for the hydrogen de- and absorption.

[1] B. Bogdanovic, M Schwickardi J. Alloys Compd., 253-254 (1997), pp. 1.

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Session Classification: Meet and Eat, Poster session