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CATALYZED H₂ SORPTION MECHANISM IN ALANATES

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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 MAIH₄ 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 experimentally determined thermodynamic data (enthalpies and entropies) of individual hydrides, MAIH₄, 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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