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Investigation of Lithium Complex Hydrides Li_2MH_5 (M = B, Al) as Hydrogen Storage materials; A theoretical study

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ABSTRACT

Lithium complex hydrides Li_2MH_5 (M= B, Al) in are potential hydrogen storage material because of their high capacity of (10, 6.5 wt. % respectively) H_2. However, their high thermodynamic stability is unfavorable for dehydrogenation processes. Understanding the bonding nature of Al-H, B-H and Li-H are essential for predicting their dehydrogenation mechanism and then improving their dehydrogenation performance. Quadrupolar parameters of nuclei can be used as a tool to understand the electronic structure of compounds. In this work the charge density distribution in Li_2AlH_5 and Li_2BH_5 was compared. Thus using calculated Nuclear Quadrupole Coupling Constants (NQCC) of ^2H nuclei, the electronic structure of Li_2AlH_5 and Li_2BH_5 was studied. The results show that between two proposed dehydrogenation mechanisms for Li_2MH_5, hetro phase dehydrogenation is preferred than partial dissociation to $LiMH_4$. Furthermore easier condition for hetro phase dehydrogenation is expected in Li_2AlH_5.

*The electric field gradient (EFG) of quadrupolar nuclei were calculated to obtain NQCC parameters. All calculations performed using Gaussian 03 at MP2/6-311G** level of theory. The selected level and basis set give the rather acceptable qualitative NQCCs of hydrogen atoms.*

Keywords: Nuclear quadrupole resonance (NQR); Lithium complex hydrides; Hydrogen; Ab initio calculations; Nuclear Quadrupole Coupling Constant (NQCC)

1. INTRODUCTION

With concerning current trends in environmental pollution and depletion of fossil energy resources, there is an imperative to seek renewable and clean energy sources that can support the continued sustainable development of human society. Hydrogen is regarded as one of the best alternative sustainable energy carriers because of its abundance, high energy density and lack of adverse environmental impact (for example, when oxidized as water).