Dehydrogenation mechanism of LiBH₄ by Poly(methyl methacrylate)

Hydrogen is considered as a promising alternative energy carrier owing to its high-energy density, abundance, light weight and pollution-free burning [1]. Developing a safe and efficient hydrogen storage material is one of the key challenges for the mobile application of hydrogen [2]. Due to the high gravimetric (18.5 wt.%) and volumetric (121 kg H₂/m³) hydrogen density, lithium borohydride (LiBH₄) has been acknowledged as a potential candidate for hydrogen storage materials [3]. However, due to the unfavorable high thermal stability (e.g. decomposition peak temperature of ~ 470 ºC), the practical utilization of LiBH₄ as hydrogen storage medium is hampered [4]. Hence, several approaches including reactant destabilization, catalyst/additive introduction, nanostructuring, and anion/cation substitution have been applied to decrease the dehydrogenation temperature and accelerate the kinetics [5].

Nanoengineering had been demonstrated to be a useful method to reduce the dehydriding/rehydridding temperature of LiBH₄ by decreasing diffusion path lengths and increasing surface areas [6]. However, nanoscale LiBH₄ is too reactive and very sensitive to the water and oxygen in the air, which impede its practical utilization. PMMA ((Poly (methyl methacrylate))), with a high permeability ratio of H₂/O₂, was reported to have good gas selectivity [7]. Therefore, in this project, PMMA was applied to protect LiBH₄ from oxygen and water but let the hydrogen get in or out freely (Scheme 1). Furthermore, the nanoconfinement of LiBH₄ in the fine network pore of PMMA and the interaction between the B atom in LiBH₄ and the O atom in C=O of PMMA resulted in a much lower hydrogen release temperature of LiBH₄. LiBH₄ PMMA composite started to dehydrogenate at 53 ºC and released 5.2 wt.% of hydrogen at 162 ºC within 1 h. This project provides a general strategy to utilize a gas-selective polymer to protect air-sensitive hydrogen storage compounds and improve their hydrogen storage properties.

![Scheme 1. Schematic illustration of LiBH₄ protected from oxygen and water by PMMA.](image)

References

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Paper Reference:
Jianmei Huag et al. (2015) “Dehydrogenation mechanism of LiBH₄ by Poly(methyl methacrylate)”
Journal of Alloys and Compounds 645 (1), S100-S102

Hidden Product:
QGA