Significantly improved de/rehydrogenation properties of lithium borohydride modified with hexagonal boron nitride

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Electronic supplementary information

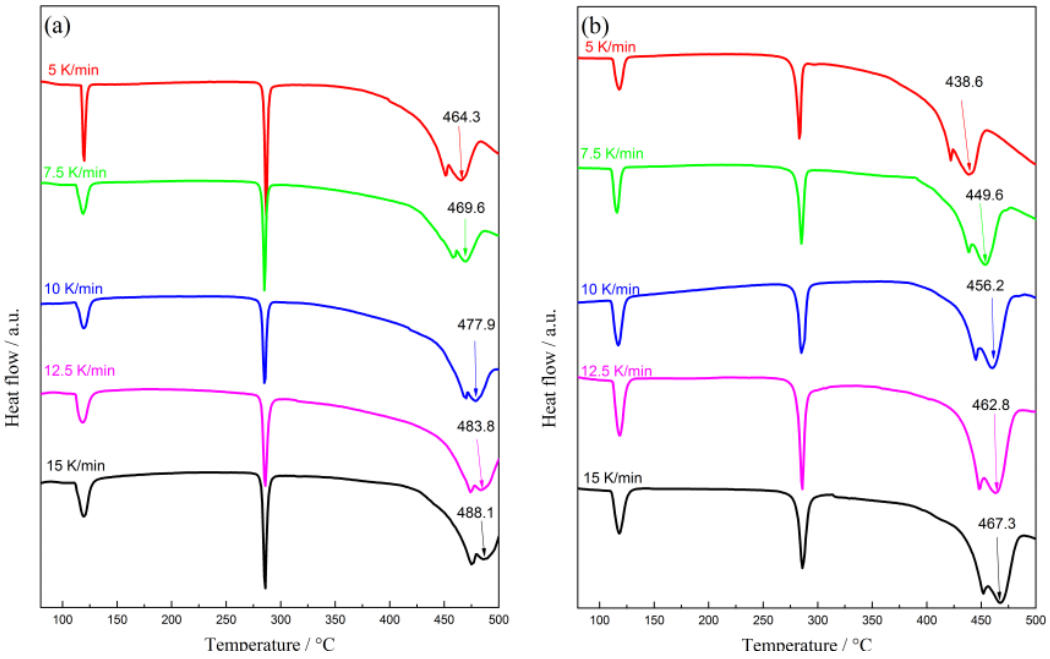

Fig.S1 DSC profiles of (a) ball milled $LiBH_4$ and (b) 30 mol% h-BN doped $LiBH_4$ samples at different heating rate.

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† Electronic Supplementary Information (ESI) available: DSC curves with different rates and Isothermal dehydrogenation curves of the $LiBH_4$ doped with graphite. See DOI: 10.1039/x0xx00000x

As both h-BN and graphite are sheet structure, the $LiBH_4$ doped with the same weight of graphite as the weight of h-BN of the 30 mol% h-BN doped $LiBH_4$ sample was prepared in the same condictions. For comparison, the isothermal dehydrogenation curves of the graphite doped $LiBH_4$ sample was displayed in the Fig. S2. The results shows that the 30 mol% h-BN doped $LiBH_4$ sample could release 12.6 wt% within 2 h, while the graphite doped $LiBH_4$ sample only release 4.6 wt% hydrogen, much better than the graphite doped $LiBH_4$ sample. The most difference between h-BN and graphite is lone pair electrons of nitrogen of h-BN, and $LiBH_4$ is an "electron-deficient" molecule, which possess fewer electrons than those apparently required to fill all the bonding orbital. So it is highly possible that the lone pair electrons of nitrogen atom on the h-BN surface may induce destabilization of $LiBH_4$ by the lone pair electrons complex with "electron-deficient" molecule $LiBH_4$.

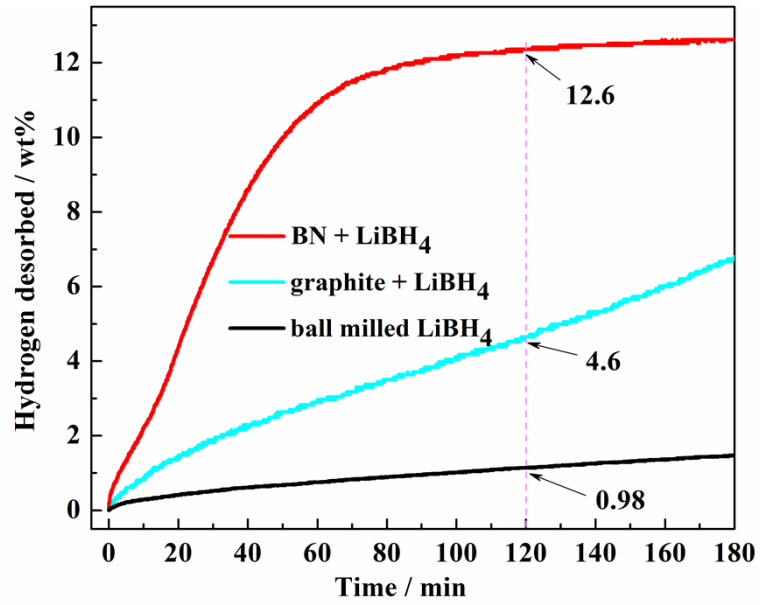

Fig. S2 the isothermal dehydrogenation curves of the ball milled $LiBH_4$, 30 mol% h-BN doped $LiBH_4$ and graphite doped $LiBH_4$ samples. Special notes: the weight of graphite additive of the graphite doped $LiBH_4$ sample is equal to the weight of h-BN of the 30 mol% h-BN doped $LiBH_4$ sample, and was prepared in the same conditions.