Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

NbN nanoparticles as additive for the high dehydrogenation properties of $LiAlH_4$

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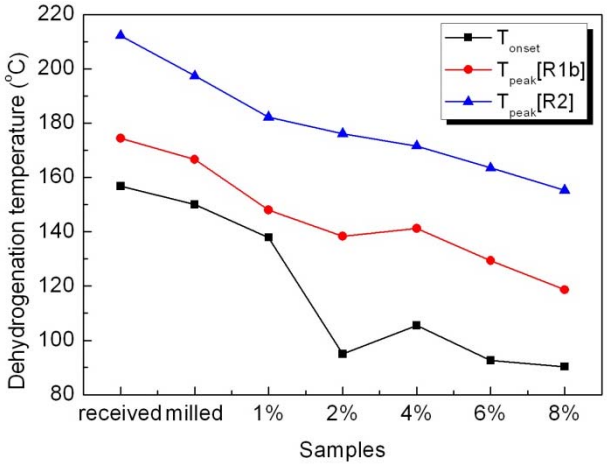

Fig. S1 The onset dehydrogenation temperature and dehydrogenation peak temperatures (R1b and R2) of DSC for as–received $LiAlH_4$ (received), as–milled $LiAlH_4$ (milled) and x%NbN–$LiAlH_4$ (x=1, 2, 4, 6 and 8) samples.

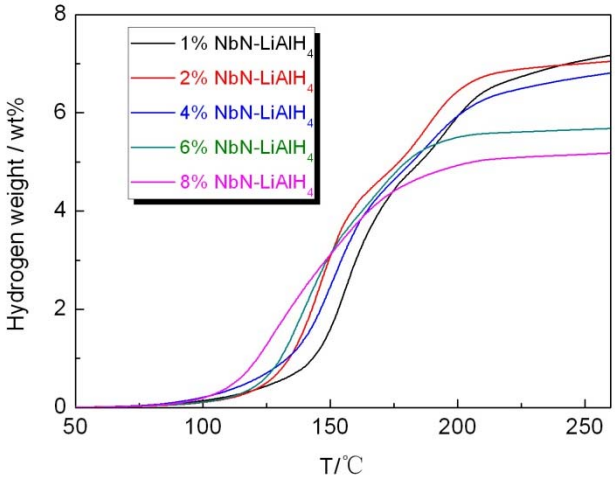

Fig.S2 Hydrogen desorption curves of 1%NbN–$LiAlH_4$, 2% NbN–$LiAlH_4$, 4% NbN–$LiAlH_4$, 6% NbN–$LiAlH_4$ and 8% NbN–$LiAlH_4$ samples after ball milling. (Heating ramp 2 °C/min)

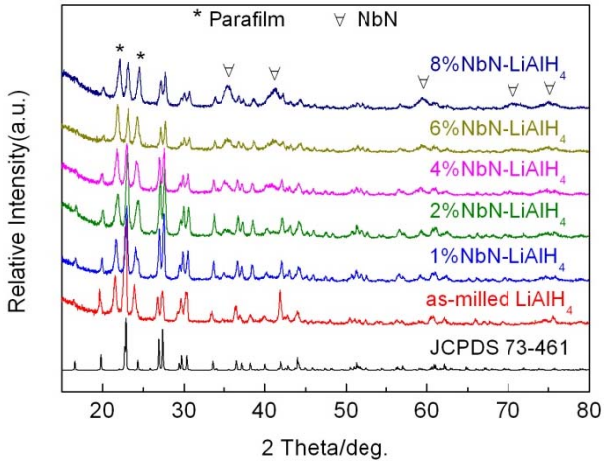

Fig. S3 XRD patterns for the as–milled $LiAlH_4$ and x%NbN–$LiAlH_4$ (x=1, 2, 4, 6 and 8) samples after ball milling.

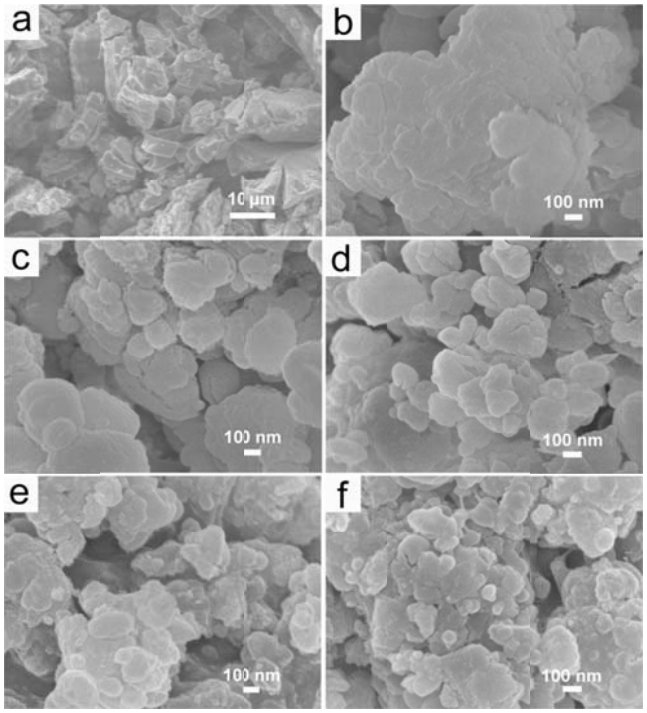

Fig. S4 SEM image of (a) as–received $LiAlH_4$ (b) 1%NbN–$LiAlH_4$, (c) 2%NbN–$LiAlH_4$, (d) 4%NbN–$LiAlH_4$, (e) 6%NbN–$LiAlH_4$ and (f) 8%NbN–$LiAlH_4$ samples after ball milling, respectively.

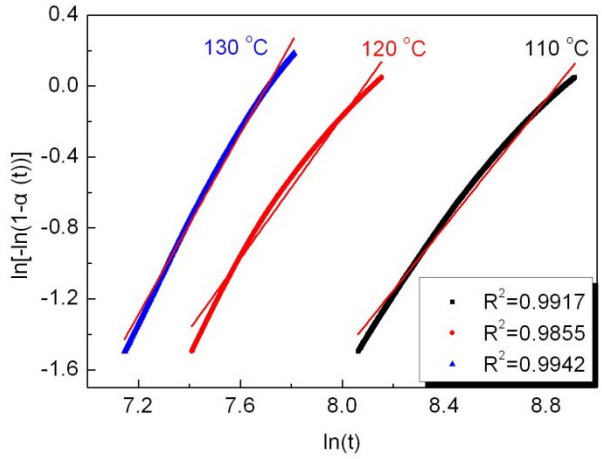

Fig. S5 JMA plots for the first-step isothermal dehydrogenation.

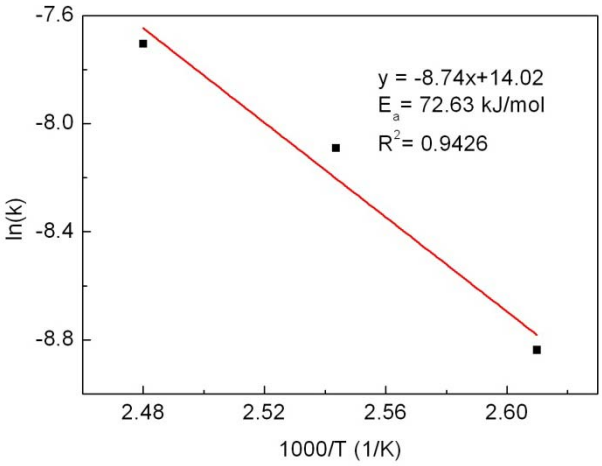

Fig. S6 Arrhenius plots for the dehydriding kinetics of NbN–$LiAlH_4$ sample.

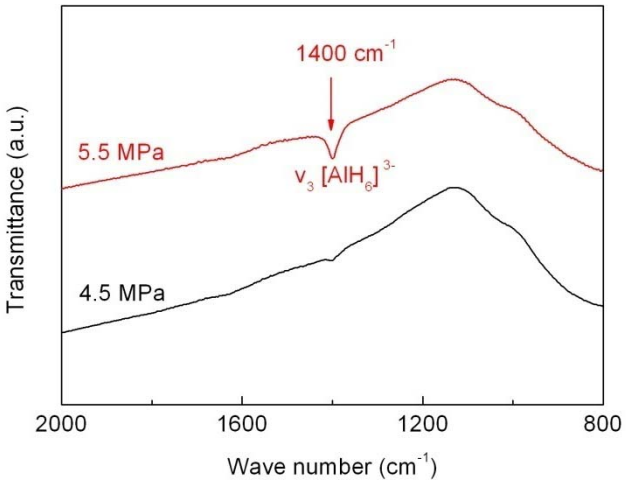

Fig. S7 FTIR spectra of the 8%NbN–$LiAlH_4$ sample after HP–DSC under 4.5 MPa and 5.5 MPa H_2.