Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Supporting Information

High catalytic efficiency of amorphous TiB_2 and NbB_2 nanoparticles for the hydrogen storage of $2LiBH_4/MgH_2$ system

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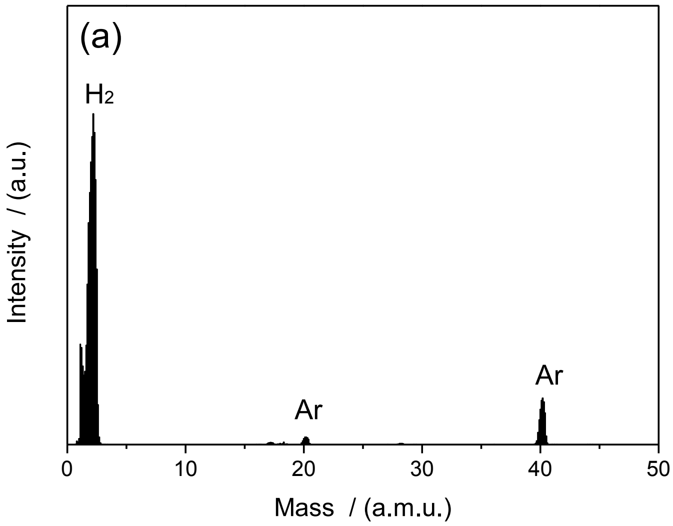


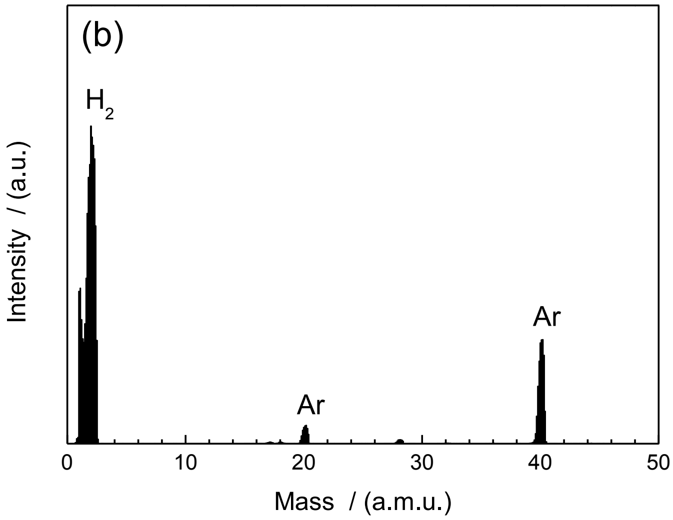


Fig. S1 Mass spectra of released gases from the mixture during ball milling: (a) for the synthesis of NbB_2; (b) for the synthesis of TiB_2.

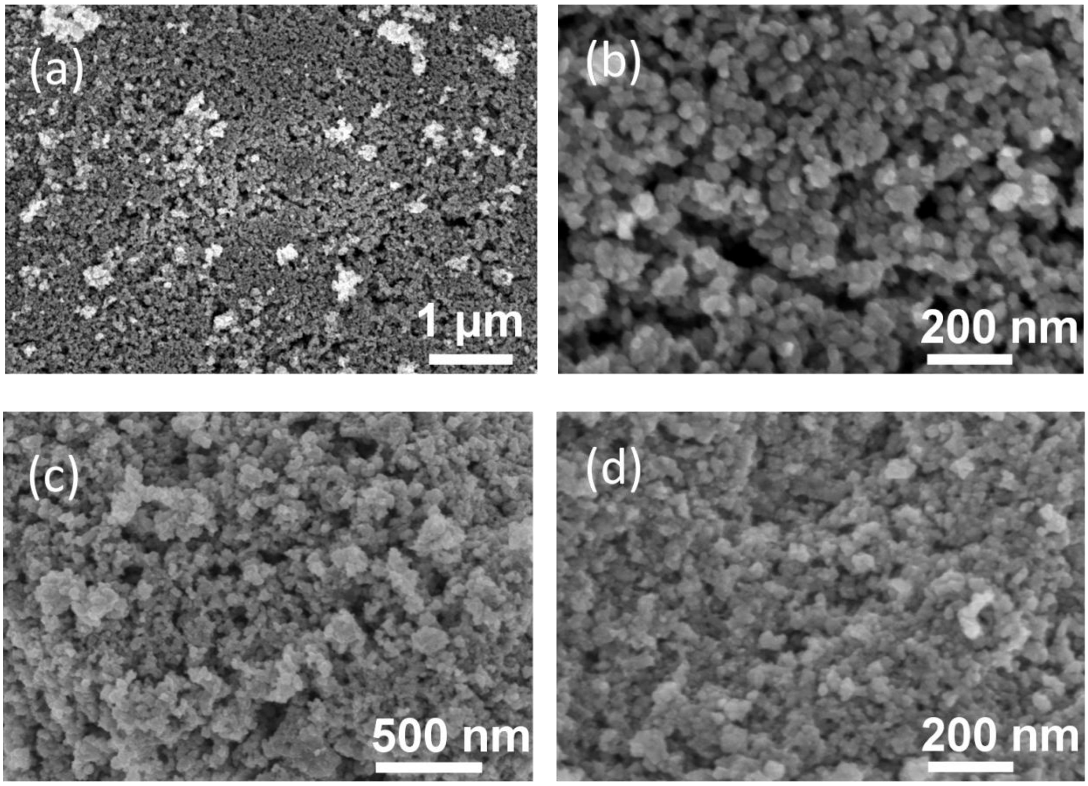


Fig. S2 SEM images of as-synthesized NbB_2 (a), (b); and TiB_2 (c), (d).

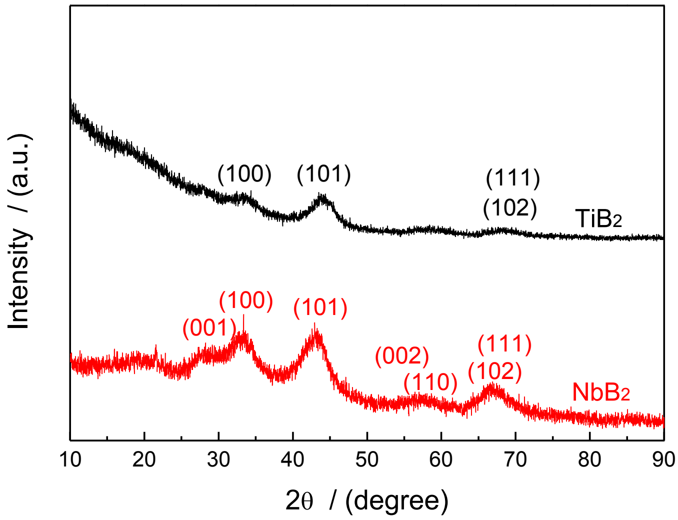
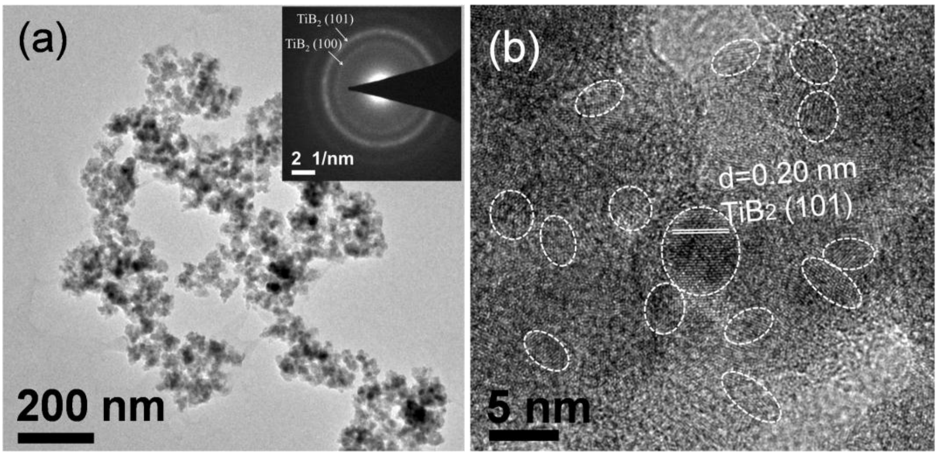


Fig. S3 XRD patterns for synthesized TiB_2 and NbB_2 after heat treatment at 700 °C for 12 h. Broad peaks indicate that nanocrystallites are formed during heat treatment.



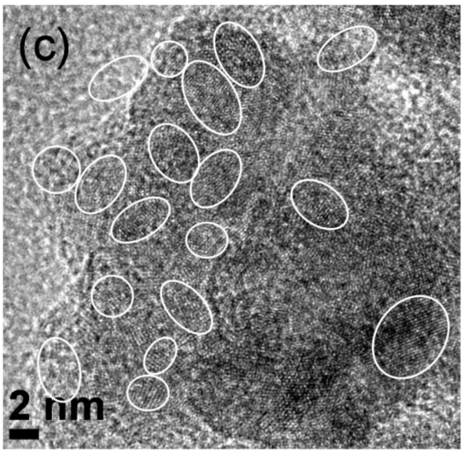
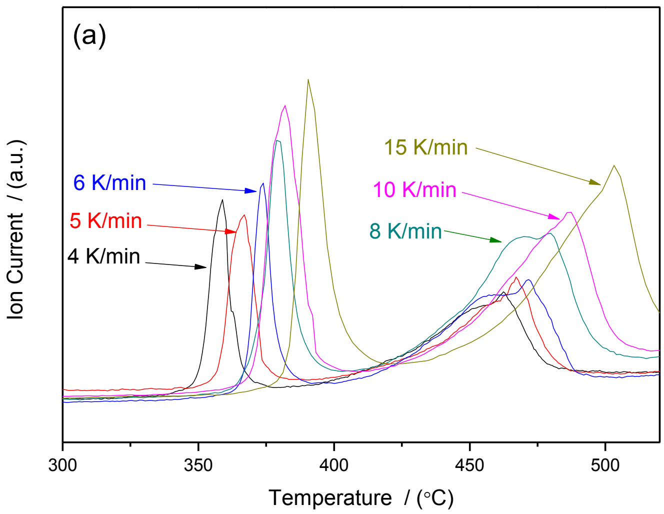
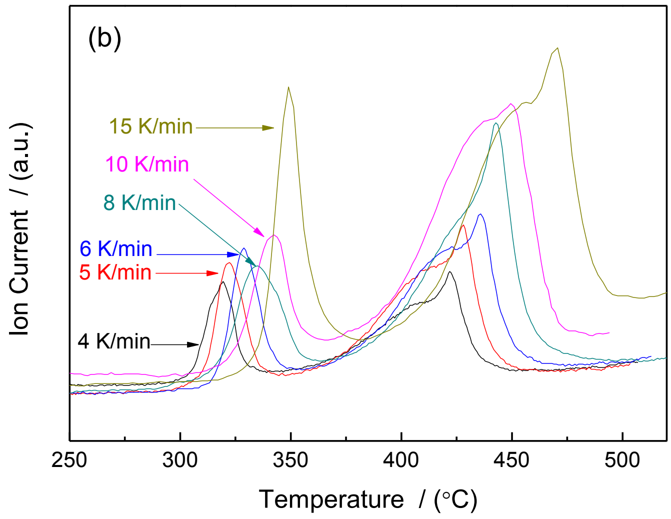


Fig. S4 TEM (a) and HRTEM (b) image for synthesized TiB_2 after heat treatment at 700 °C for 12 h, HRTEM (c) image for synthesized NbB_2 after heat treatment at 700 °C for 12 h. The inset in (a) is the corresponding SAED, which exhibits a conventional diffraction rings of a nanocrystalline phase. Uniform nanocrystallites with size of ~ 3 nm can be observed in (b) and (c).





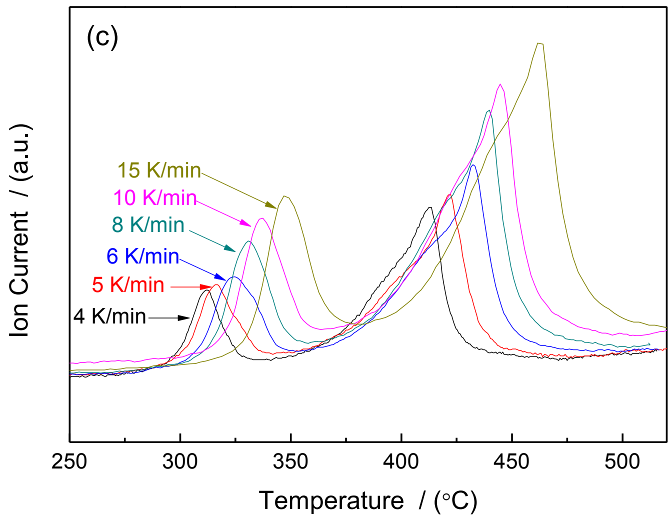


Fig. S5 MS spectra of the $2LiBH_4/MgH_2$ composite: (a) undoped; (b) doped with nanoNbB_2; (c) doped with nanoTiB_2.

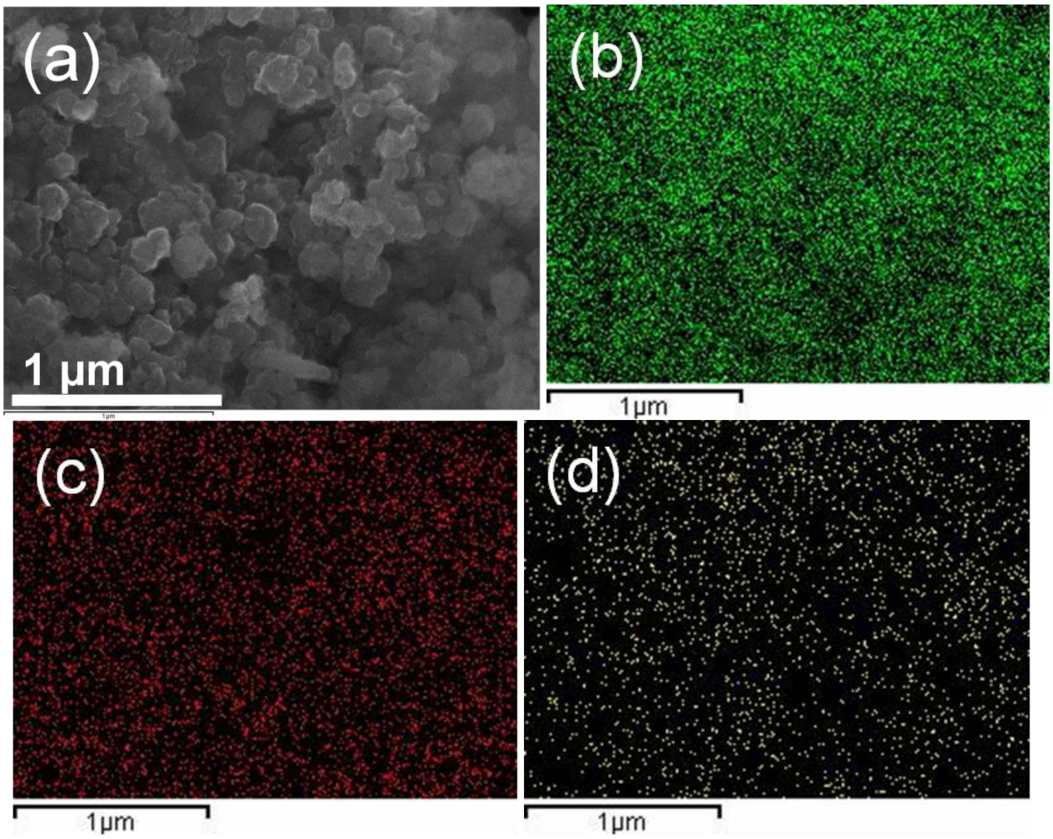


Fig. S6. SEM image (a) and corresponding EDS maps of Mg (b), B (c) and Ti (d) for the nanoTiB_2 doped $2LiBH_4/MgH_2$ after dehydrogenation in the 3rd cycle. The elements of Mg, B and Ti exhibit a homogeneous dispersion in the composite.

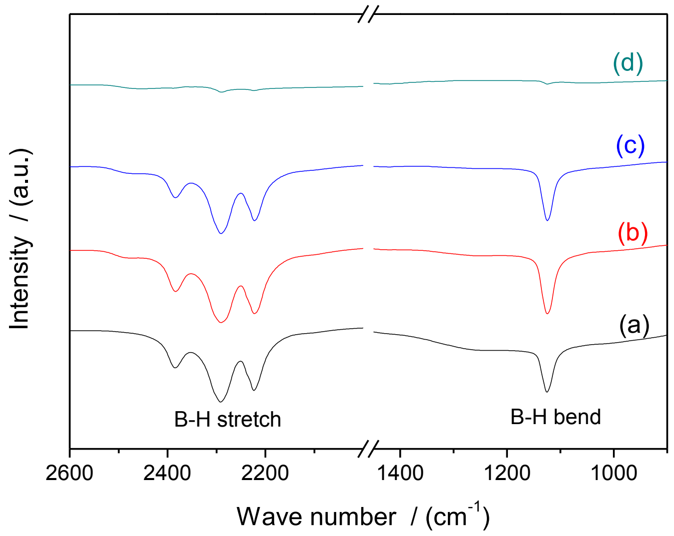


Fig. S7 FTIR spectra of nanoTiB$_2$-doped 2LiBH$_4$/MgH$_2$: (a) after ball milling; (b) after hydrogenation of 3rd cycle; (c) after hydrogenation of 5th cycle; (d) after dehydrogenation of 6th cycle at 400 °C.