Supplementary information

A GBH/$LiBH_4$ coordination system with favorable dehydrogenation

Yanhui Guo,[a] Qinfen Gu,[b] Zaiping Guo,[c] Jianfeng Mao,[c] Huakun Liu,[c] Shixue Dou[c] and Xuebin Yu*[a, c]

[a] Department of Material Science, Fudan University, Shanghai 200433, China
[b] Australian Synchrotron Company Ltd, Victoria 3168, Australia
[c] Institute for Superconducting and Electronic Materials, University of Wollongong, NSW 2522, Australia

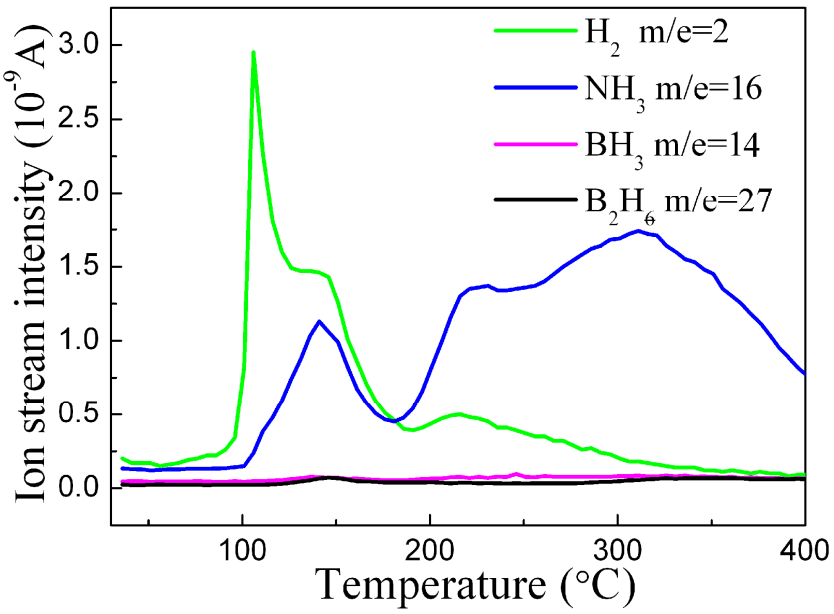
E-mail: yuxuebin@fudan.edu.cn

Table S1 Atomic coordinates following refinement of GBH/$LiBH_4$ (S1)

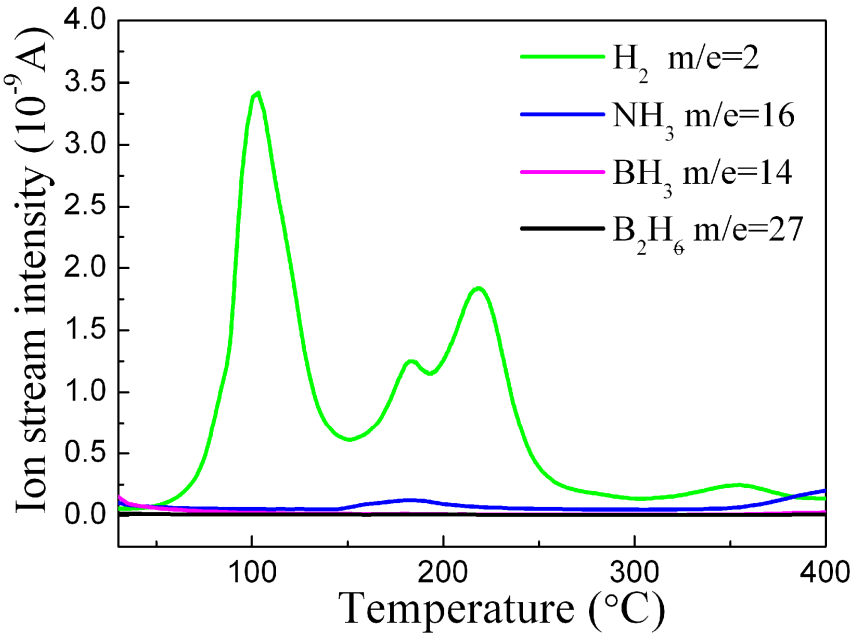
Atom	Wyck.	x/a	y/b	z/c
Li1	2a	0.3942(19)	0.4436(58)	0.5683(26)
Li2	2a	0.3991(18)	0.5818(34)	0.0901(27)
Li3	2a	0.2159(25)	0.0960(35)	0.8655(22)
Li4	2a	0.6626(18)	0.9749(38)	0.2895(19)
B21	2a	0.6100(5)	0.6794(9)	0.9269(5)
H21a	2a	0.53864	0.64197	0.89879
H21b	2a	0.63208	0.69681	1.02014
H21c	2a	0.64305	0.55182	0.89809
H21d	2a	0.62110	0.82884	0.88796
B22	2a	0.5687(6)	0.7254(6)	0.2312(2)
H22a	2a	0.50258	0.65276	0.21324
H22b	2a	0.57424	0.78433	0.15011
H22c	2a	0.57478	0.85003	0.29368
H22d	2a	0.61963	0.60548	0.26662
B23	2a	0.1022(8)	0.7668(5)	0.4138(4)
H23a	2a	0.10441	0.82445	0.32957
H23b	2a	0.13405	0.88703	0.47801
H23c	2a	0.03409	0.74059	0.40664
H23d	2a	0.13824	0.61656	0.43549
B24	2a	0.2477(5)	0.7184(1)	0.2817(8)
H24a	2a	0.21460	0.87068	0.24760
H24b	2a	0.31586	0.72855	0.28133
H24c	2a	0.24286	0.69654	0.36653
H24d	2a	0.21455	0.58642	0.22710
B25	2a	0.5660(4)	0.2523(1)	0.7150(2)
H25a	2a	0.60174	0.40573	0.73771

H25b	2a	0.58144	0.18603	0.64143
H25c	2a	0.58679	0.15085	0.78961
H25d	2a	0.49508	0.27960	0.69177
B26	2a	0.2674(9)	0.2352(4)	0.4490(2)
H26a	2a	0.28776	0.25929	0.54308
H26b	2a	0.22861	0.37370	0.40828
H26c	2a	0.32656	0.21493	0.42566
H26d	2a	0.22705	0.09170	0.42566
B27	2a	0.7843(1)	0.2645(3)	0.9226(6)
H27a	2a	0.84861	0.22899	0.98804
H27b	2a	0.79670	0.30043	0.84218
H27c	2a	0.74231	0.12759	0.91669
H27d	2a	0.75414	0.40291	0.94920
B28	2a	0.7410(8)	0.7263(8)	0.7510(1)
H28a	2a	0.72353	0.61166	0.80879
H28b	2a	0.81043	0.76913	0.79013
H28c	2a	0.72786	0.65069	0.66852
H28d	2a	0.70047	0.86948	0.74148
C1	2a	0.4883(8)	0.7549(7)	0.5035(6)
N1a	2a	0.44758	0.92045	0.47885
H1a	2a	0.39747	0.91890	0.43827
H1b	2a	0.40300	0.58564	0.42607
N1b	2a	0.45311	0.58717	0.46665
H1c	2a	0.47083	1.03105	0.50318
H1d	2a	0.48001	0.47811	0.48294
N1c	2a	0.56448	0.75733	0.56519
H1e	2a	0.58513	0.64950	0.57650
H1f	2a	0.58153	0.86633	0.58443
C2	2a	0.8519(2)	0.2488(5)	0.6830(2)
N2a	2a	0.89255	0.08237	0.70114
H2a	2a	0.87468	-0.01805	0.66050
H2b	2a	0.76632	0.16234	0.56258
N2b	2a	0.78418	0.26276	0.60322
H2c	2a	0.93720	0.07317	0.75375
H2d	2a	0.75741	0.37247	0.59128
N2c	2a	0.87906	0.40127	0.74473
H2e	2a	0.85053	0.49774	0.72817
H2f	2a	0.92103	0.38036	0.79187
C3	2a	0.8655(5)	0.7629(9)	0.1849(9)
N3a	2a	0.78789	0.75427	0.13002
H3a	2a	0.76224	0.64332	0.12298
H3b	2a	0.87861	0.49234	0.22225

N3b	2a	0.90427	0.60327	0.22930
H3c	2a	0.76237	0.85954	0.10082
H3d	2a	0.95546	0.60903	0.26554
N3c	2a	0.90450	0.93145	0.19568
H3e	2a	0.95201	0.92408	0.23062
H3f	2a	0.87629	1.02230	0.16603
C4	2a	0.9969(8)	0.7936(8)	0.9969(6)
N4a	2a	1.03606	0.92531	0.95935
H4a	2a	1.08869	0.92502	0.97955
H4b	2a	1.09047	0.66119	1.08532
N4b	2a	1.03784	0.66147	1.06513
H4c	2a	1.00914	1.01241	0.91439
H4d	2a	1.01208	0.57466	1.08988
N4c	2a	0.91707	0.79406	0.96624
H4e	2a	0.89784	0.70834	0.99304
H4f	2a	0.89669	0.87999	0.92423



(a)



(b)

Fig. S1. Mass spectrometry (MS) analysis of GBH (a) and the GBH/2LiBH$_4$ (b) composite.

The figure shows that GBH undergoes an apparent two-step ammonia release, the first occurring at temperatures from 100 to 180 °C and the second from 180 to 400 °C, while only a trace of ammonia release can be observed from GBH/2LiBH$_4$ over the same temperature range, indicating a significant improvement in the suppression of NH_3 release from the GBH/2LiBH$_4$.

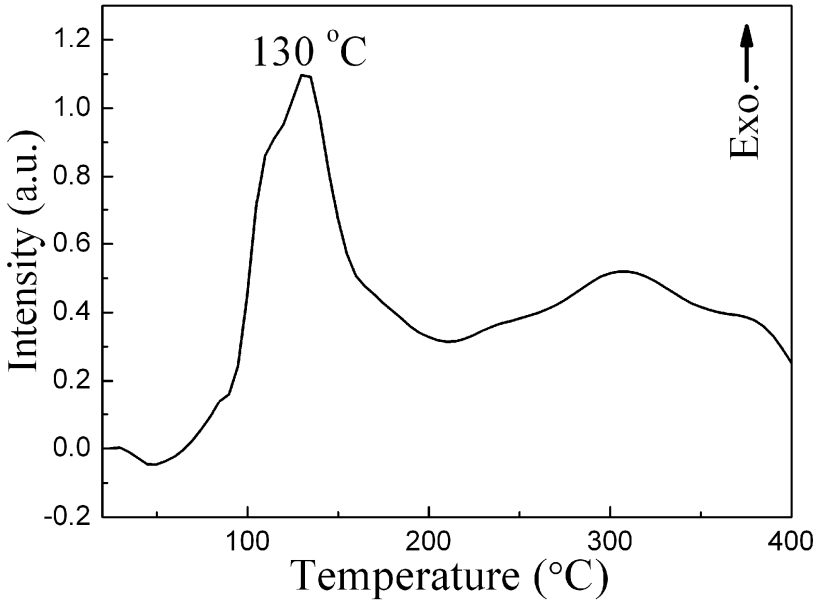


Fig. S2. DTA results for GBH / $2LiBH_4$.

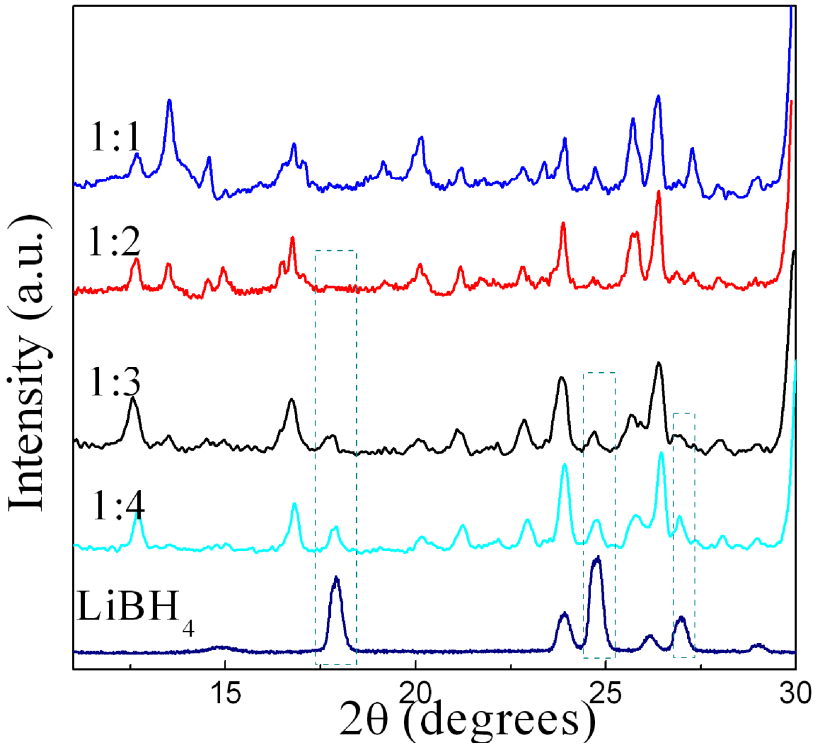


Fig. S3. XRD patterns of $LiBH_4$ and GBH/$LiBH_4$ compositions with various mole ratios.

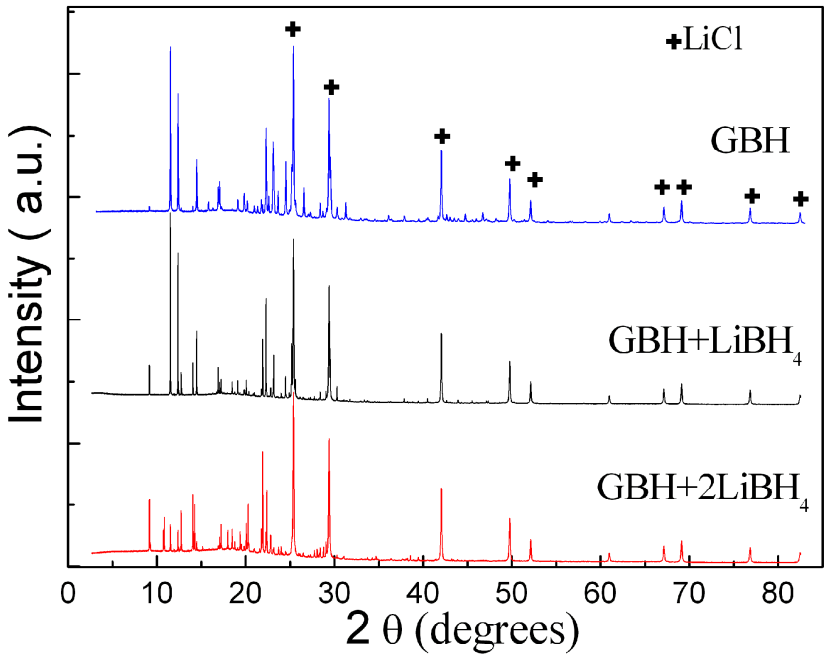


Fig. S4. Comparison of calculated XRD patterns of GBH, $LiBH_4$ with high-resolution XRD patterns of GBH/$LiBH_4$ and GBH/2$LiBH_4$.

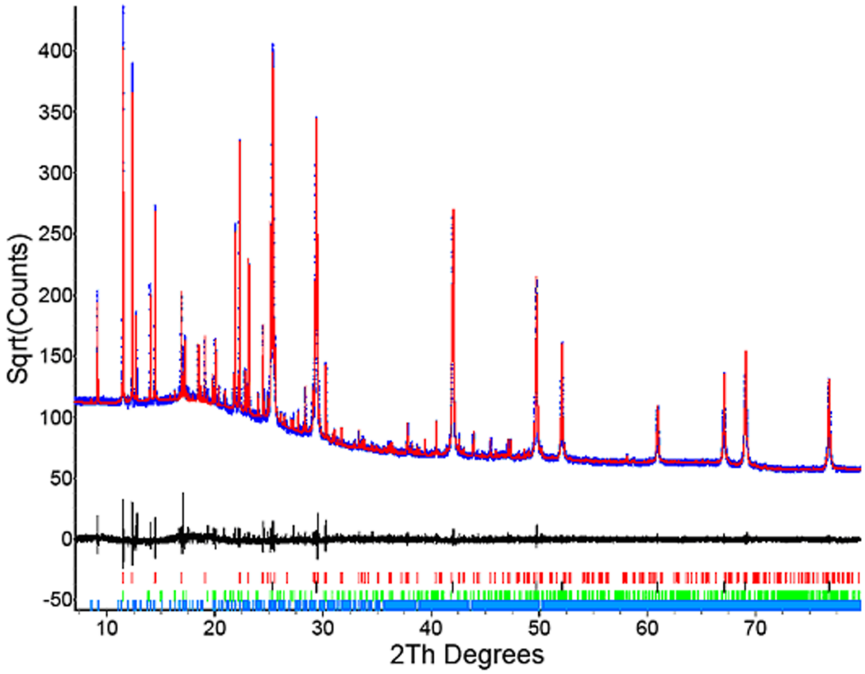


Fig. S5. Rietveld refinement profile for GBH/$LiBH_4$ phase showing observed (blue), calculated (red), difference (black) plots. The position of Bragg reflections (tick marks) from top to bottom are shown for GBH, LiCl, $C(NH_2)_3Cl$, and $LiC(NH_2)_3(BH_4)_2$. A small amount of unreacted $C(NH_2)_3Cl$ is observed in the sample due to an incomplete solid state reaction.

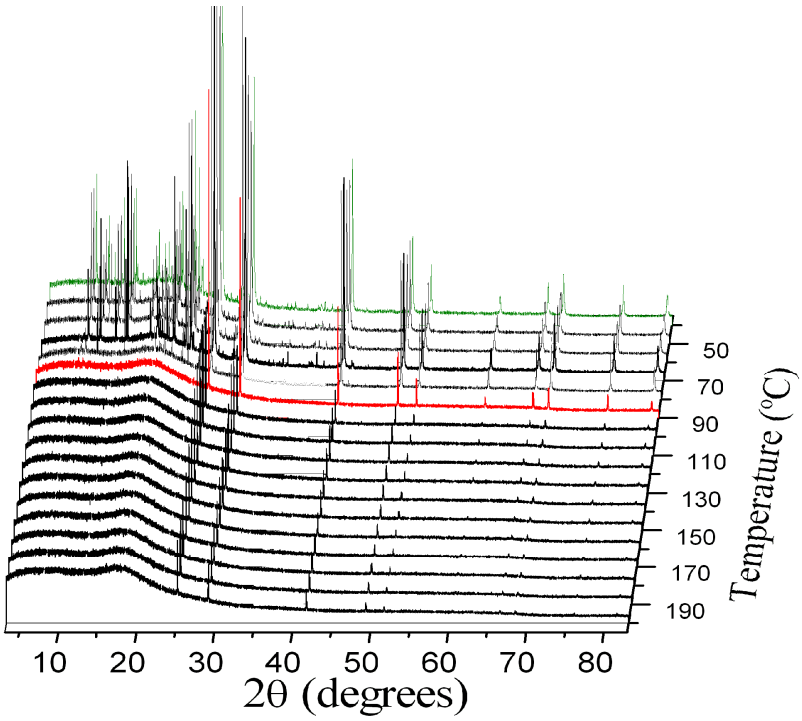


Fig. S6. (a) *In-situ* high-resolution XRD patterns for GBH/2LiBH$_4$ composite. (b) selected part of (a).