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Supporting Information

for

Realizing Facile Regeneration of $NaBH_4$ by Mg-Al Alloy

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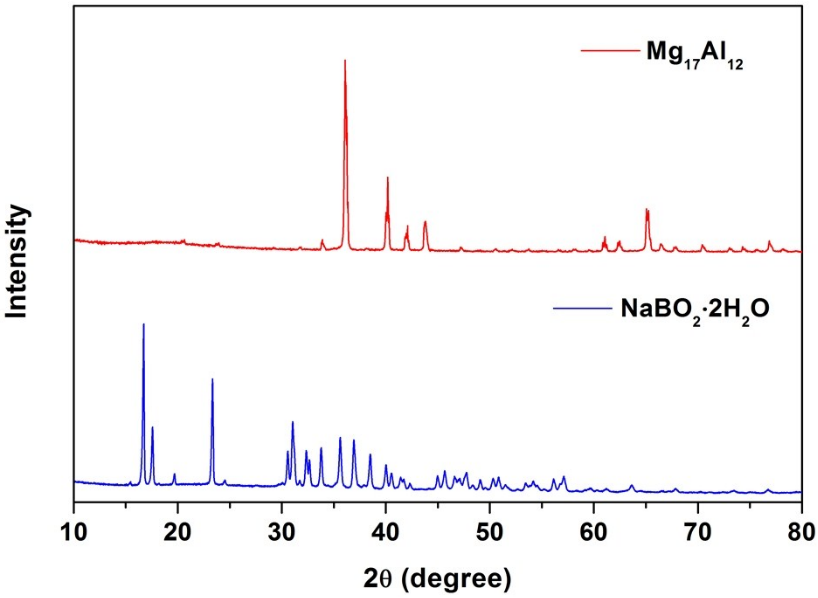

Fig. S1 XRD patterns of the raw materials: $Mg_{17}Al_{12}$ (red line) and $NaB(OH)_4$ (blue line).

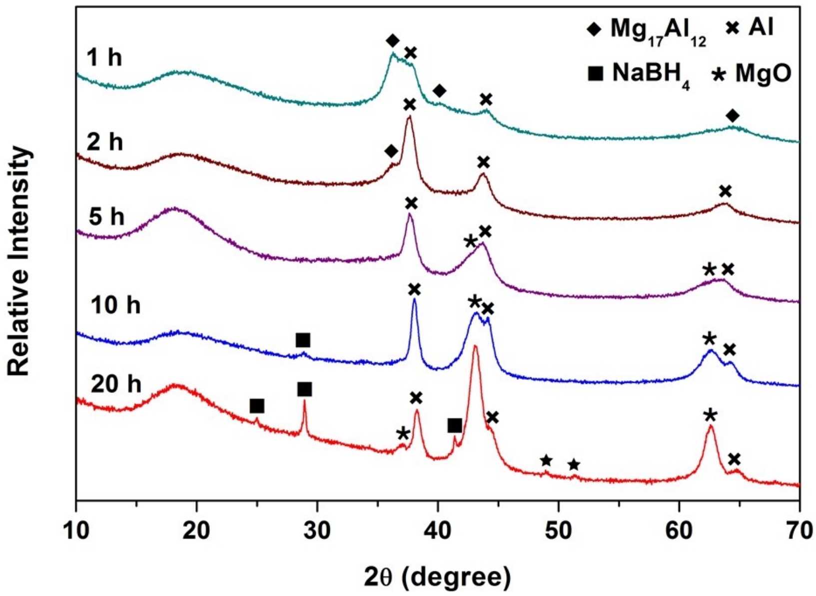

Fig. S2 XRD patterns of the 1, 2, 5, 10 and 20 h ball milled products of $Mg_{17}Al_{12}$ and $NaB(OH)_4$ (in a 4: 17 mole ratio).

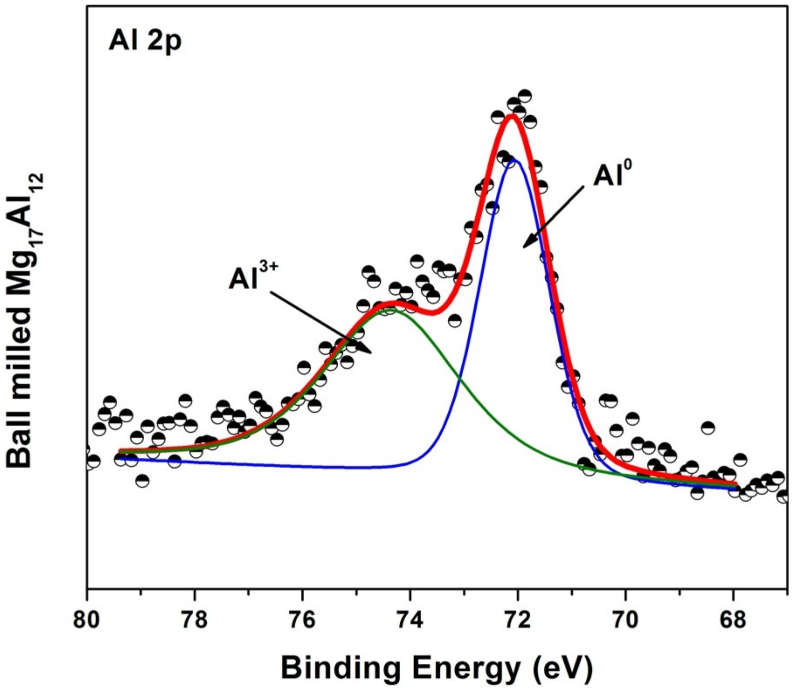

Fig. S3 XPS spectra of Al 2p of the 1 h ball milled products of pure $Mg_{17}Al_{12}$.

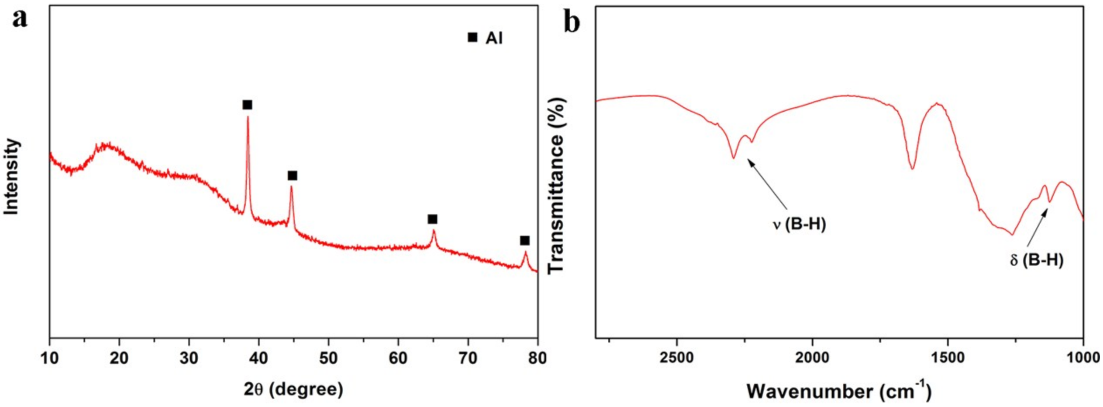

Fig. S4 (a) XRD pattern of the 5 h ball milled product of Al and $NaB(OH)_4$ with a mole ratio of 24:9.

Table S1. Reaction mechanism, yield, optimal reaction condition and cost calculation of raw materials for $NaBH_4$ produced by different approaches.

Reactants	Reaction mechanism	Yield	Cost (US $/ ton)	Optimal reaction condition
$Mg_{17}Al_{12}$, $NaB(OH)_4$	Hydrogen in $NaB(OH)_4$ transforms to H^- via the reaction with $Mg_{17}Al_{12}$ and produce $NaBH_4$, MgO and Al_2O_3.	72%	14,550 [a)]	Raw materials mole ratio is 4 : 17; ball milling time is 20 h.
MgH_2, $NaBO_2$	Hydrogen from MgH_2 transfer to $NaBO_2$ and produce $NaBH_4$ and MgO.	76%	280,630 [b)]	Raw materials mole ratio is 2.8 : 1; ball milling time is 6 h.
NaH, $B(OCH_3)_3$ (commercial method)	Via a heating treatment, hydrogen from NaH substitutes the $[(OCH_3)_3]^{3-}$ and produce $NaBH_4$ and $NaOCH_3$.	99.5%	18,670 [c)]	With a $B(OCH_3)_3$ excess of 6.5 folds.
Mg, $NaB(OH)_4$ [6]	Hydrogen in $NaB(OH)_4$ transforms to H^- via the reaction with Mg and produces $NaBH_4$ and MgO.	68%	10,072 [6]	Raw materials mole ratio is 5.5: 1; ball milling time is 15 h.
Al, H_2, NaOH, $NaBO_2$	Hydrogen from H_2 transforms to H^- via the reaction between Al and $NaBO_2$ and produces $NaBH_4$ and Al_2O_3. In this process Na_2O reacts with Al_2O_3 to produce porous $NaAlO_2$ for the continuously reaction.	65%	497,750 [d)]	Mole ratio of Al, H_2, NaOH and $NaBO_2$ is 4: 6: 4: 3. The reaction is operating under 23 bar H_2 pressure at 853 K.

[a)] According to our manuscript, a $NaBH_4$ yield of 37% can be achieved by ball milling $Mg_{17}Al_{12}$ and $NaBO_2 \cdot 2H_2O$ with a 4: 35 mole ratio. Thus about 6 tons of $Mg_{17}Al_{12}$ can produce 1 ton $NaBH_4$. Since the price of $Mg_{17}Al_{12}$ is \$2420/ ton, the total cost of raw materials is \$14550; [b)] In the reaction between MgH_2 and $NaBO_2$, MgH_2 and $NaBO_2$ with a ratio of 2: 1 can generate $NaBH_4$ with a yield of 63% [1]. About 2.21 tons of MgH_2 can thus produce 1 ton $NaBH_4$. Because the price of MgH_2 is \$127,000/ ton, then the total cost of raw materials is \$280,630; [c)] Supposed by a yield of 100 % in current industrial production, 4.23 tons of NaH are needed for production of 1 ton $NaBH_4$. The price of NaH is \$4413, then the total cost of raw materials is \$18,670. All the price of raw materials is from the same commercial company[2] The commercial method for $NaBH_4$ production is based on the Brown-Schlesinger process [3] and the Bayer process.[4, 5] [d)] In the reaction between Al, H_2, Na_2O and $NaBO_2$ with a ratio of 4: 6: 4: 3 can generate $NaBH_4$ with a yield of 65% [7]. Therefore, about 1.46 tons of Al and 2.17 tons of NaOH can produce 1 ton $NaBH_4$. Because the price of Al is \$2,065/ ton, while NaOH is \$450/ ton, then the total cost of solid raw materials is \$2515. In addition, 1822000 Nm^3 hydrogen is used to produce $NaBH_4$. Considering renewable hydrogen used in this method, the price of hydrogen is about \$0.27/ Nm^3,[8] thus the cost of renewable hydrogen is \$493,740. The total cost of the raw materials is \$497,750.

The costs of the electricity consumption are not taken into account in this case, because the electricity price depends on many factors such as production time, location, electric power company, etc. In some locations e.g. California the electricity price produced from regenerative sources becomes negative at certain times.[9] This makes electricity costs of the process less important. Therefore we have not considered electricity costs for the calculation.

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