Supporting Information

Hamamelis-like $K_2Ti_6O_{13}$ Synthesized by Alkali Treatment of Ti_3C_2 MXene: Catalysis for Hydrogen Storage in MgH_2

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Supplementary materials

Materials: All chemical reagents were purchased from commercial suppliers and used without further purification. MgH_2 was purchased from Aldrich and used as received. TiH_2 (99 wt.% purity, 325 mesh), Al (99.9 wt.% purity, 200-400 mesh), Graphite (99.95 wt.% purity, ≥325 mesh) and HF (49 wt.%) were purchased from Aladdin and were used as received. potassium hydroxide (KOH, Shanxitongjie Chemical Reagent Co., Ltd., ACS, 82 wt.%), hydrogen peroxide (H_2O_2, Luoyang Chemical Reagent Co., Ltd., ACS, 30 wt.%), ethanol solution (Sinopharm Chemical Reagent Co., Ltd., AR), distilled water.

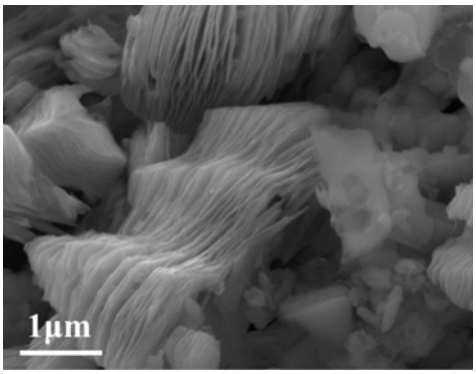

Figure S1. SEM image of the Ti_3C_2 sample.

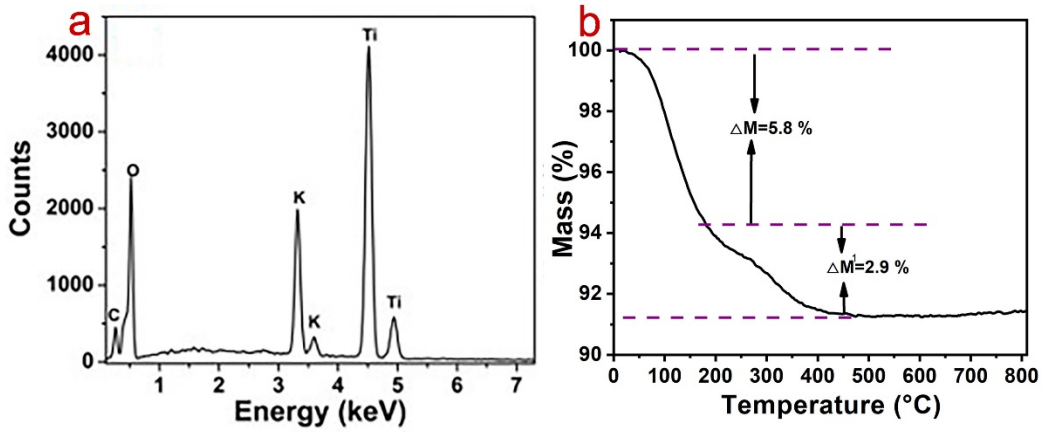

Figure S2. (a) Elemental analysis, (b) TGA of $K_2Ti_6O_{13}$ sample.

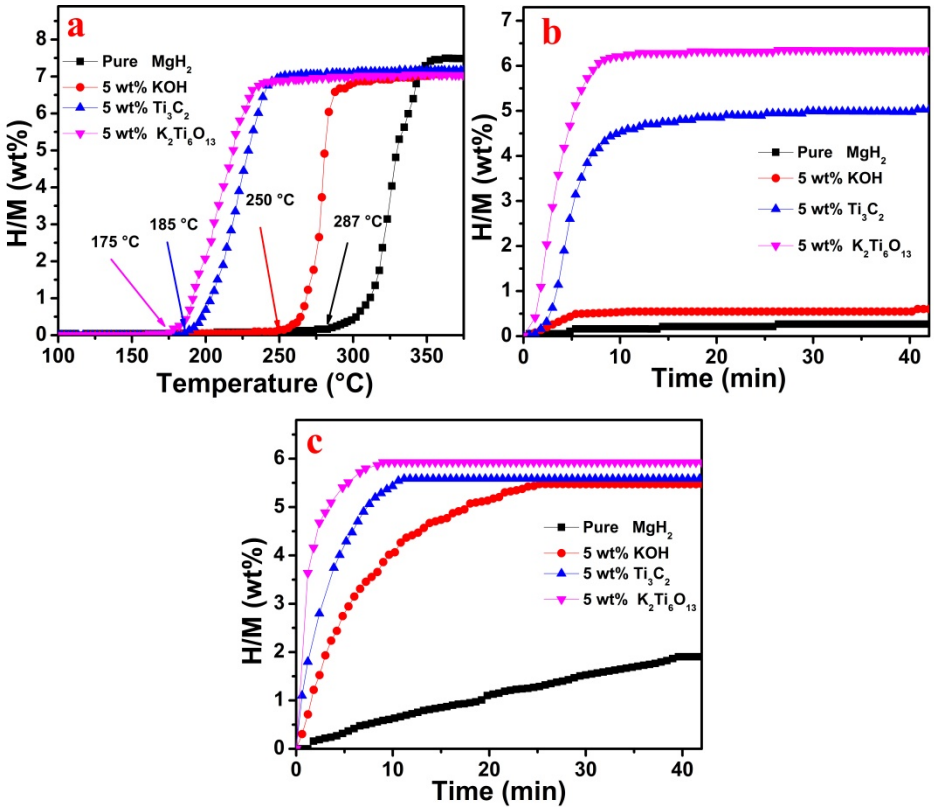

Figure S3. (a) TPD profiles, (b) isothermal dehydrogenation curves at 240 °C, (c) isothermal hydrogenation curves at 150 °C of the pure MgH_2, 5 wt % KOH, 5 wt % Ti_3C_2, 5 wt % $K_2Ti_6O_{13}$ samples.

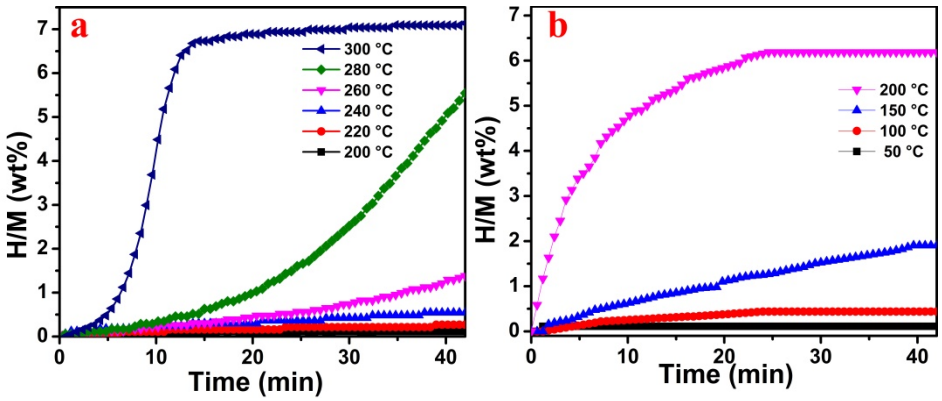

Figure S4. (a) Isothermal dehydrogenation, (b) isothermal hydrogenation curves of the pristine MgH_2 sample.

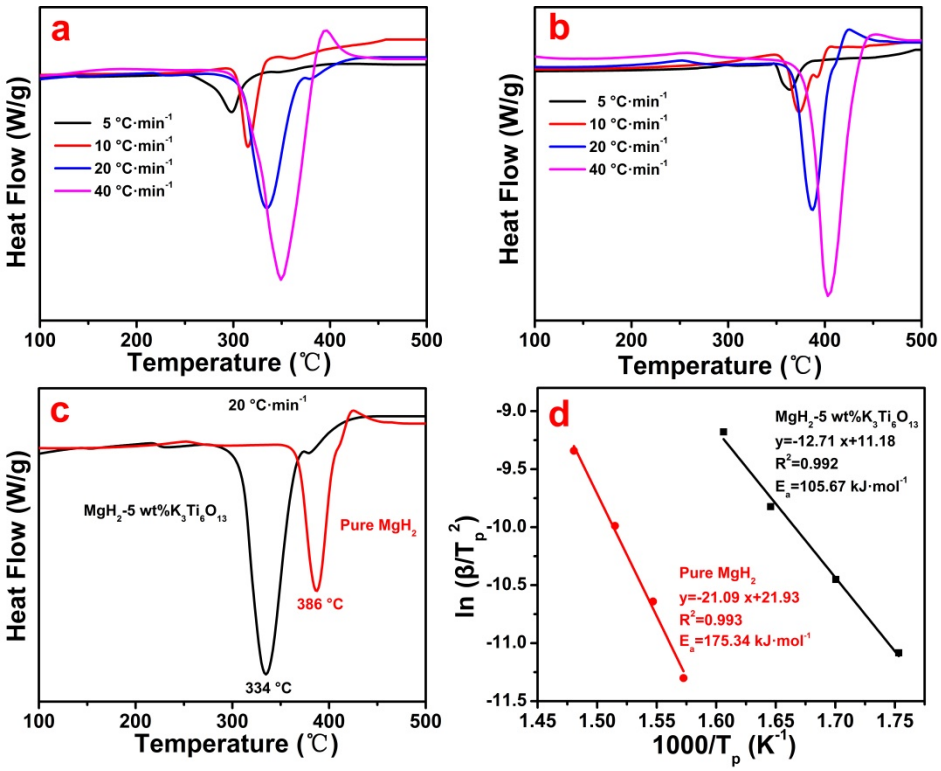

Figure S5. DSC curves of (a) MgH_2-5 wt% $K_2Ti_6O_{13}$, (b) pure MgH_2 at different heating rates, (c) MgH_2-5 wt% $K_2Ti_6O_{13}$ and pure MgH_2 at 20 °C min^{-1}. (d) Kissinger plots of MgH_2-5 wt% $K_2Ti_6O_{13}$ and pure MgH_2.

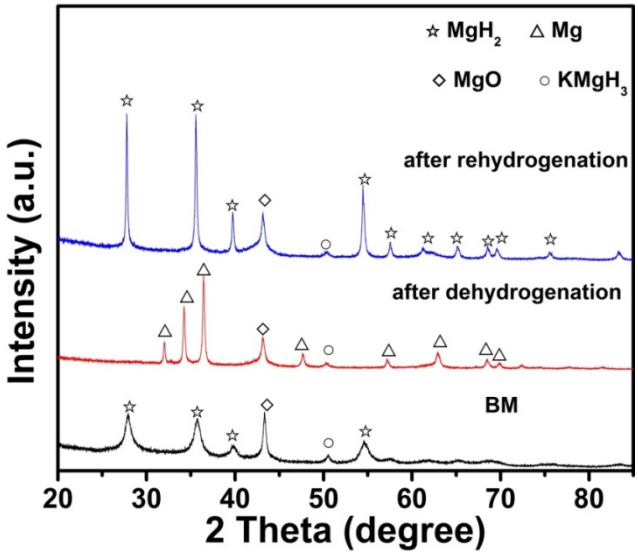

Figure S6. XRD pattern of the as-milled MgH_2-20 wt % $K_2Ti_6O_{13}$ sample milled, after hydrogenation and after dehydrogenation.

Table S1. Common solid-state rate expressions for different reaction models

symbol	model	f(α)	Sharp's expression
D1	one-dimensional diffusion	α^2	$0.2500(t/t_{0.5})$
D2	two-dimensional diffusion	$\alpha+ (1- \alpha)\ln(1- \alpha)$	$0.1534(t/t_{0.5})$
D3	three-dimensional diffusion	$[1-(1- \alpha)^{1/3}]^2$	$0.0426(t/t_{0.5})$
D4	three-dimensional diffusion (Ginstling- Braunsshtein equation)	$(1- 2\alpha/3)- (1- \alpha)^{2/3}$	$0.0367(t/t_{0.5})$
F1	first-order reaction	$-\ln(1- \alpha)$	$-0.6931(t/t_{0.5})$
R2	two-dimension phase boundary	$1-(1- \alpha)^{1/2}$	$0.2929(t/t_{0.5})$
R3	three-dimension phase boundary	$1-(1- \alpha)^{1/3}$	$0.2063(t/t_{0.5})$
A2	Avarami-Erofe'ev	$[-\ln(1- \alpha)]^{1/2}$	$0.8326(t/t_{0.5})$
A3	Avarami-Erofe'ev	$[-\ln(1- \alpha)]^{1/3}$	$0.8850(t/t_{0.5})$

Table S2. Comparison of dehydrogenation/hydrogenation kinetics of MgH_2 with various catalysts.

Additive	Initial temperature (°C)	dehydrogenation	hydrogenation	E_a ($kJ \cdot mol^{-1}$)	Ref.
$K_2Ti_6O_{13}$	175	6.7 wt% - 3 min-280 °C	6.5 wt% - 30 s – 200 °C	105	This work
$Na_2Ti_3O_7$ nanotubes	--	6.5 wt% - 6 min-300 °C	6.0 wt% - 60 s – 275 °C	70.43	S1
$Na_2Ti_3O_7$ nanorods	--	6.5 wt% - 6 min-300 °C	--	164.84	S1
$BaTiO_3$	270	3.341 wt% - 21 s-350 °C	2.245 wt% - 21 min – 150 °C	108	S2
$SrTiO_3$	275	5.2 wt% - 340 °C	4.3 wt% - 60 min – 320 °C	109	S3
TiN@rGO	167	6.0 wt% - 18 min – 300 °C	--	120	S4
TiF_3-SWCNTs	260	6.3 wt% - 23 min - 300 °C	5.5 wt% - 20 min - 270 °C	--	S5
TiB_2-GNSs	--	6.5 wt% - 40 min – 300 °C	--	90.8	S6
TiH_2	--	--	4.8 wt% - 10min – 300 °C	--	S7
TiC	--	6.2 wt% - 33 min – 300 °C	5.1 wt% - 50 min – 200 °C	144.62	S8
Ti_3C_2	185	6.2 wt%- 1 min - 300 °C	6.1 wt% - 30 s-200 °C	98.9	S9

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