**Supporting information**

# Excellent catalysis of $TiO_2$ nanosheets with high-surface-energy {001} facets on hydrogen storage properties of $MgH_2$

Meng Zhang[a], Xuezhang Xiao[a,c,*], Xinwei Wang[a], Man Chen[a], Yunhao Lu[a,*], Meijia Liu[a], Lixin Chen [a,b,*]

[a] State Key Laboratory of Silicon Materials; School of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, China,

[b] Key Laboratory of Advanced Materials and Applications for Batteries of Zhejiang Province, Hangzhou 310013, China

[c] Guangdong Provincial Key Laboratory of Advance Energy Storage Materials, South China University of Technology, Guangzhou 510640, China

[*]Corresponding author. Tel./fax: +8657187951152.
*E-mail address*: xzxiao@zju.edu.cn (X.Z. Xiao); luyh@zju.edu.cn (Y.H. Lu); lxchen@zju.edu.cn (L.X. Chen).

The desorption energy ($E_d$) of one H atom desorbing from $(MgH_2)_3$/A-$TiO_2$ is defined as,

$$E_d = E + \frac{1}{2}E_{H2} - E'$$

where $E$ and $E'$ are the total energy after and before desorbing H. $E_{H2}$ is the total energy of the $H_2$ molecule. The lower the value, the easier it is for hydrogen desorption.

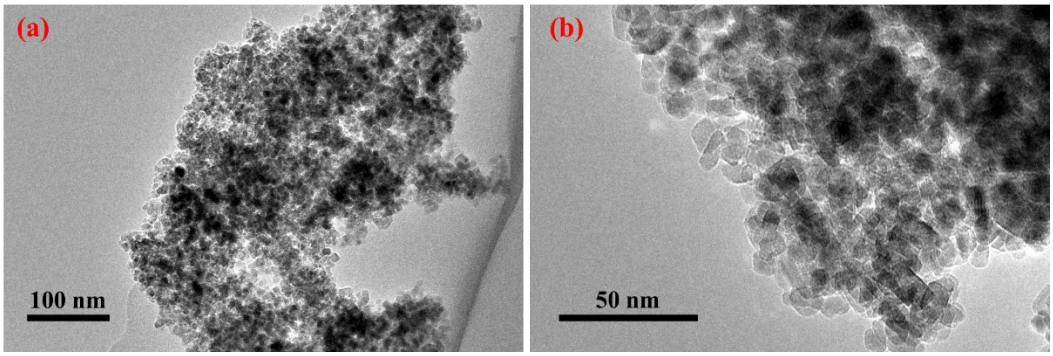


**Fig. S1** TEM images of $TiO_2$ nanoparticles.

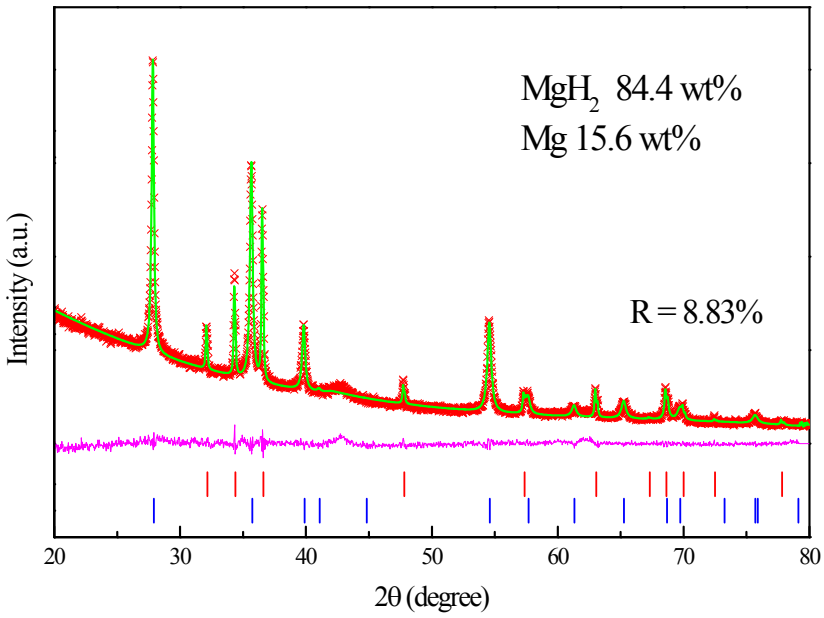


**Fig. S2** Rietveld profile plot for $MgH_2$ + 5 wt% $TiO_2$ NS sample after dehydrogenation for 12 h at 180°C. Observed (crosses), calculated (solid line) and difference curves (bottom line) are shown. Vertical bars (|) correspond to Bragg positions for Mg and $MgH_2$ phases (from top to bottom).

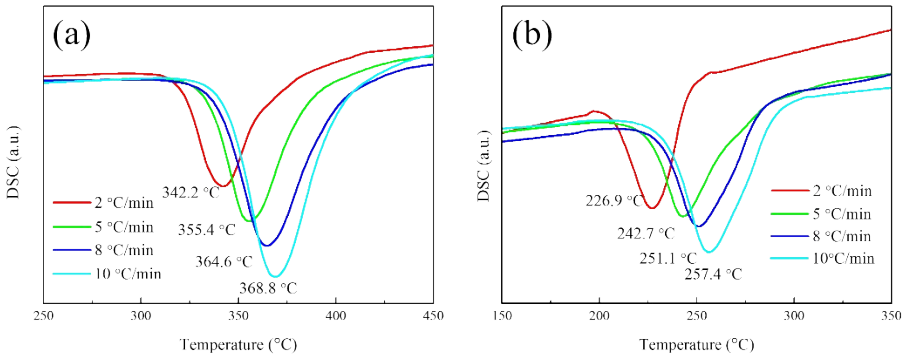


**Fig. S3** DSC profiles of (a) ball milled $MgH_2$ and (b) $MgH_2$+ 5 wt% $TiO_2$ NS samples at various heating rates(2, 5, 8 and 10 °C $min^{-1}$)

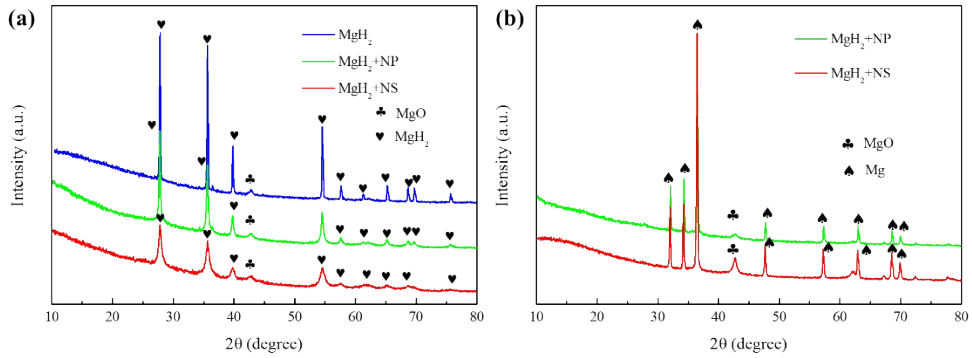


**Fig. S4** (a) XRD patterns of as-prepared $MgH_2$, $MgH_2$+$TiO_2$ NP, $MgH_2$+$TiO_2$ NS, (b) XRD patterns of $MgH_2$+$TiO_2$ NP, $MgH_2$+$TiO_2$ NS after full dehydrogenation.

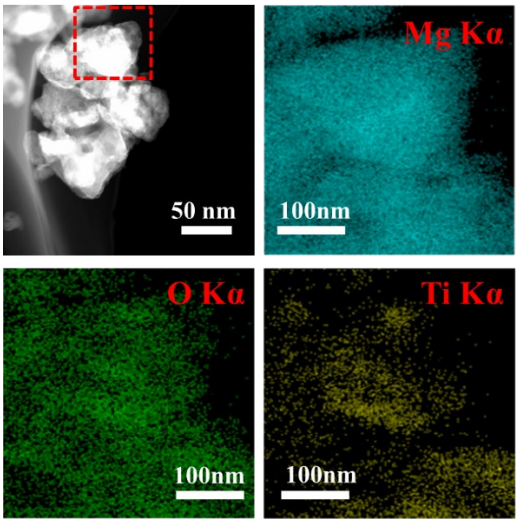


**Fig. S5** EDS mapping of as-prepared $MgH_2$ + $TiO_2$ NS.