

Electronic Supplementary Material

A striking catalytic effect of facile synthesized ZrMn₂ nanoparticles on the de/rehydrogenation properties of MgH₂

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Table S1 The bond distance and the Mulliken charge of Mg-H₂ before and after adsorption on ZrMn₂(112) surface.

	Mg-H1	Mg-H2	Mg	H1	H2
Before	1.716	1.716	0.555	0.277	0.278
After	2.626	2.847	0.498	0.072	0.012
	2.236	2.657	0.553	0.089	0.039

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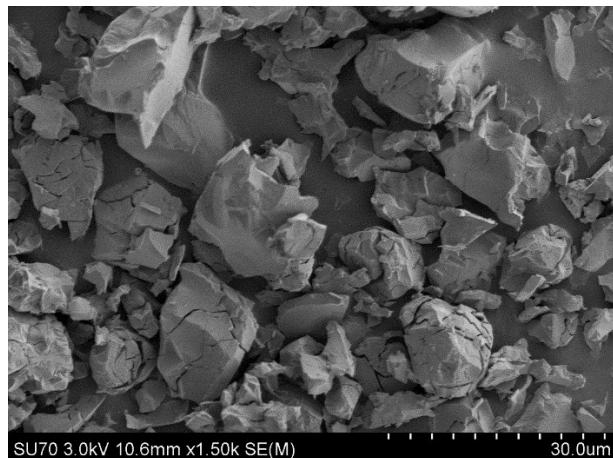


Fig. S1 SEM image of ZrMn₂ microparticles.

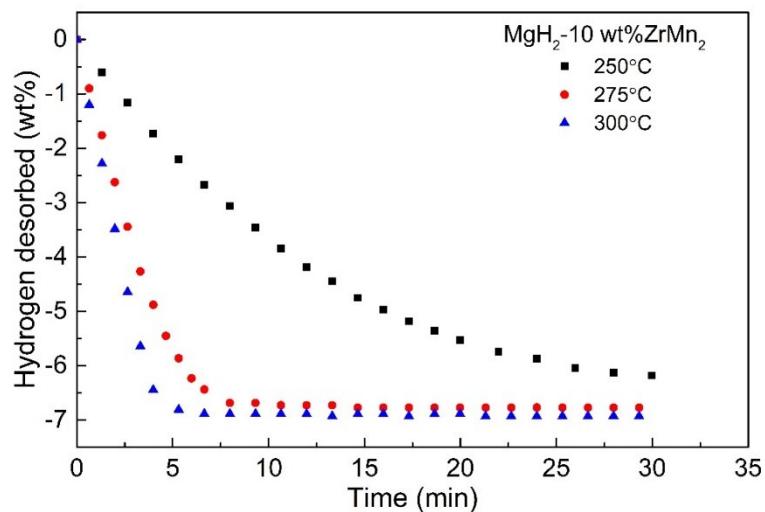


Fig. S2 Isothermal dehydrogenation curves of the MgH₂-10 wt% nano-ZrMn₂.

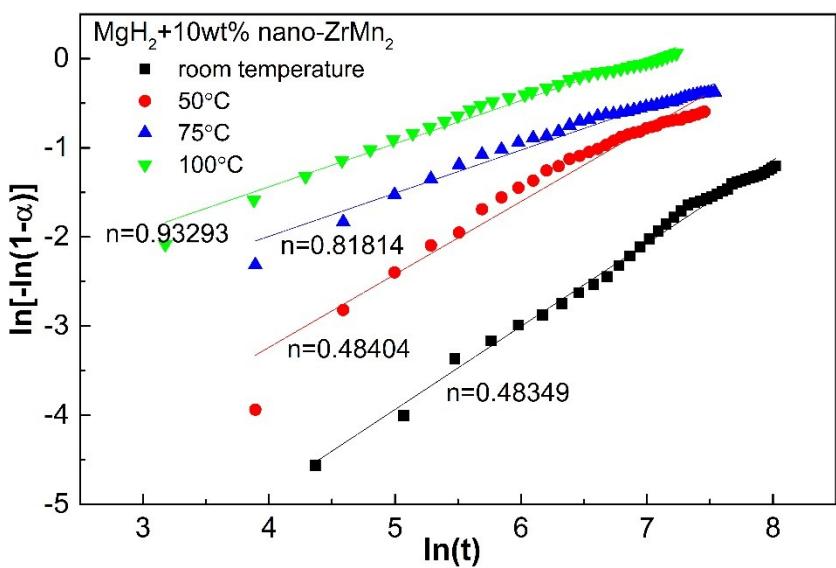


Fig. S3 JMAK plots of MgH₂+10 wt% nano-ZrMn₂ composite.

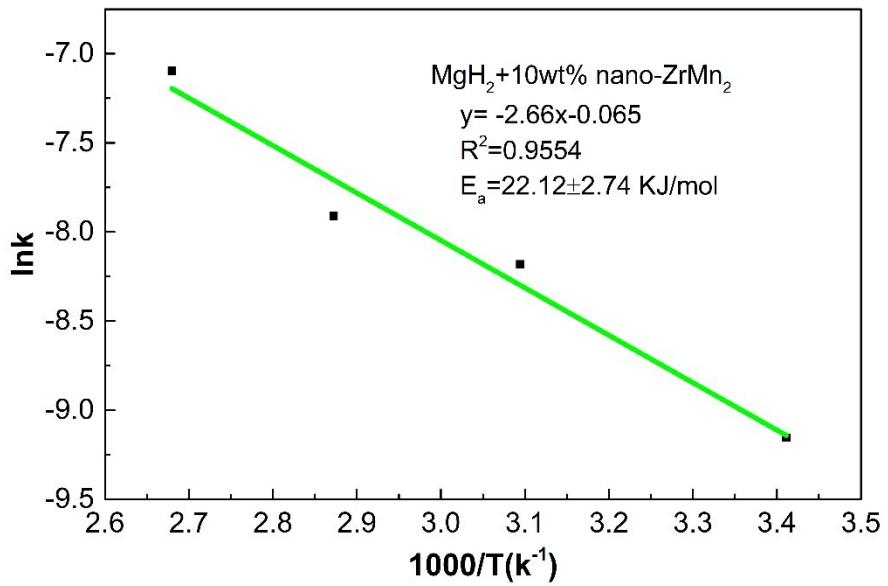


Fig. S4 Corresponding Arrhenius plots of MgH₂-10 wt% nano-ZrMn₂ composite.

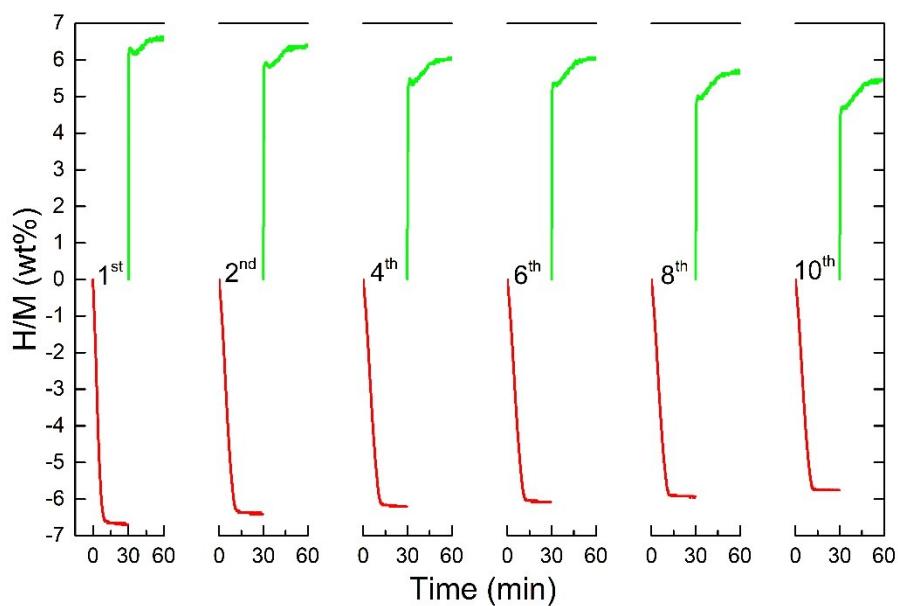


Fig. S5 Isothermal hydrogenation and dehydrogenation curves of the $\text{MgH}_2 + 10\text{wt\%}$ nano- ZrMn_2 composite as a function of cycle (green for rehydrogenation and red for dehydrogenation).

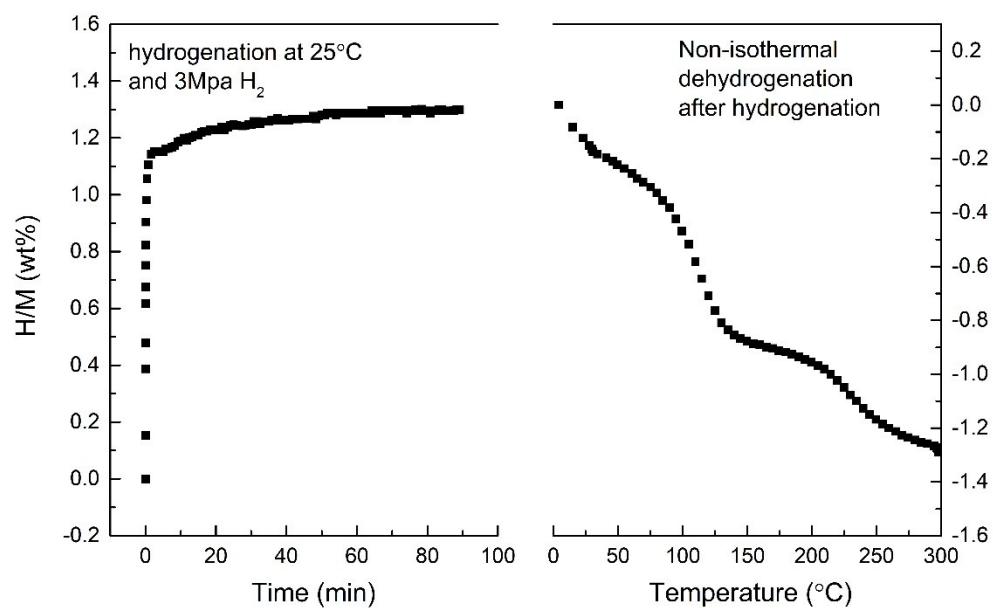


Fig. S6 Isothermal hydrogenation and non-isothermal dehydrogenation ($2 \text{ }^\circ\text{C min}^{-1}$) curves of ZrMn_2 nanoparticles.