

## Electronic Supplementary Information

### In-situ catalyzed and nanoconfined magnesium hydride nanocrystals in a Ni-MOF scaffold for hydrogen storage

Zhewen Ma <sup>a</sup>, Qiuyu Zhang <sup>a,b,c</sup>, Subrata Panda <sup>a,b,c</sup>, Wen Zhu <sup>a</sup>, Fengzhan Sun <sup>a</sup>, Darvish Khan <sup>a</sup>,  
Jinjian Dong <sup>a</sup>, Wenjiang Ding <sup>a,b,c</sup>, Jianxin Zou <sup>a,b,c\*</sup>

<sup>a</sup> National Engineering Research Center of Light Alloys Net Forming & State Key Laboratory of Metal Matrix Composites, Shanghai Jiao Tong University, Shanghai, 200240, PR China;

<sup>b</sup> Shanghai Engineering Research Center of Mg Materials and Applications & School of Materials Science and Engineering, Shanghai Jiao Tong University, Shanghai, 200240, PR China

<sup>c</sup> Center of Hydrogen Science, Shanghai Jiao Tong University, Shanghai, 200240, PR China

### Supplementary Figures:

---

\*Corresponding author: Email: [zoujx@sjtu.edu.cn](mailto:zoujx@sjtu.edu.cn); Tel.: +86 21 54742381; Fax: +86 21 34203730.

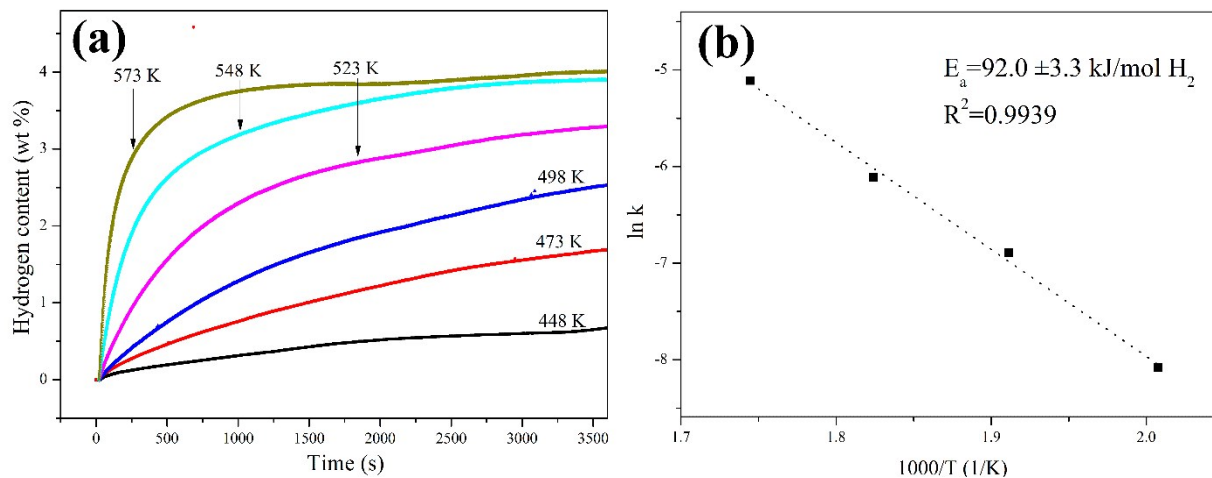


Fig. S1 (a) Isothermal hydriding profiles of the pure  $MgH_2$  (derived from  $MgBu_2$ ) and (b) the corresponding  $\ln k$  vs  $1000/T$  plot.

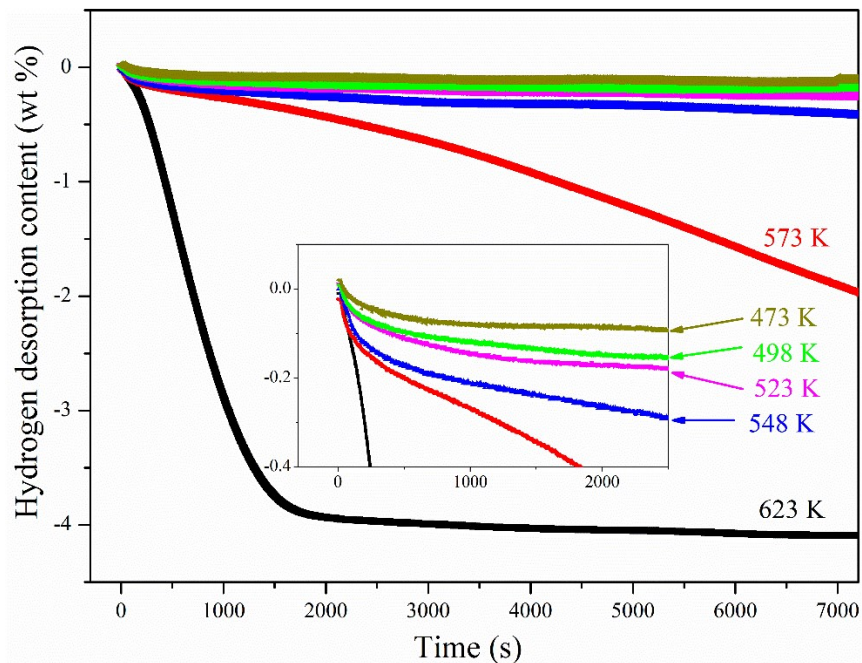


Fig. S2 Isothermal dehydriding profiles of the pure  $MgH_2$  (derived from  $MgBu_2$ ).

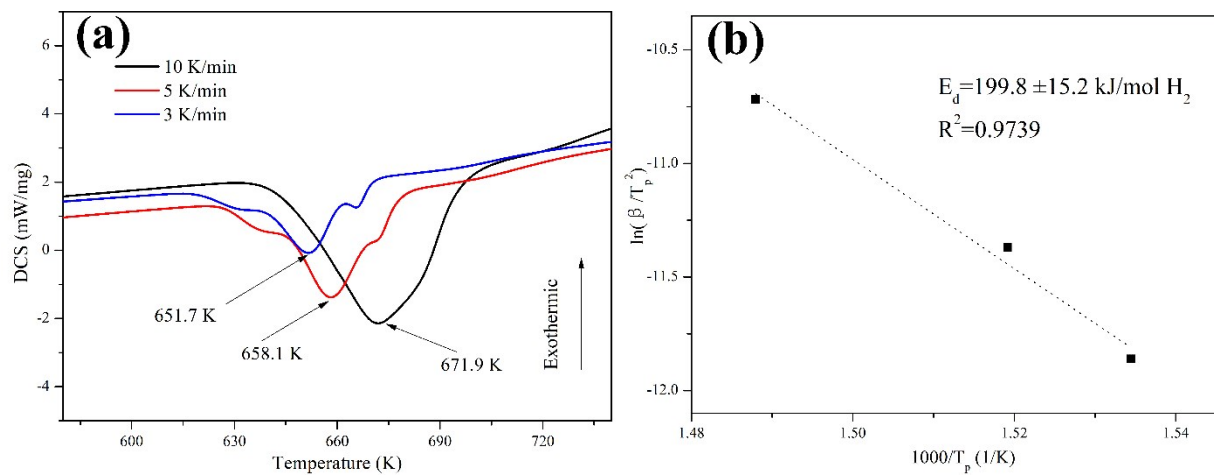


Fig. S3 (a) DSC curves obtained at different heating rates for the pure MgH<sub>2</sub> (derived from MgBu<sub>2</sub>) and (b) the corresponding  $\ln(\beta/T_p^2)$  vs  $1000/T_p$  plot.

**Supplementary Tables:**

Table S1 Pore structural parameters of the Ni-MOF scaffold determined by the N<sub>2</sub> sorption isotherms.

Sample	BET surface area (m <sup>2</sup> g <sup>-1</sup> )	Langmuir surface area (m <sup>2</sup> g <sup>-1</sup> )	BJH average pore size (nm)	Pore volume (cm <sup>3</sup> g <sup>-1</sup> )
Ni-MOF	773.46	921.67	7.58	0.4617

Table S2 PCT parameters at different temperatures subtracted from the PCT isotherms of MgH<sub>2</sub>@Ni-MOF composite.

Sample	Temperature (K)	Hydrogen absorption capacity (wt%)	Hydrogen desorption capacity (wt%)	Absorption plateaus pressure (MPa)	Desorption plateaus pressure (MPa)
MgH <sub>2</sub> @Ni-MOF	598	4.03	3.94	0.47	0.35
	623	4.02	3.91	0.85	0.64
	648	3.95	3.87	1.31	1.11
	673	4.08	3.97	2.08	1.68