

## Enhanced hydrogen storage property of $\text{MgH}_2$ by the nanocatalyst $\text{BaCrO}_4$

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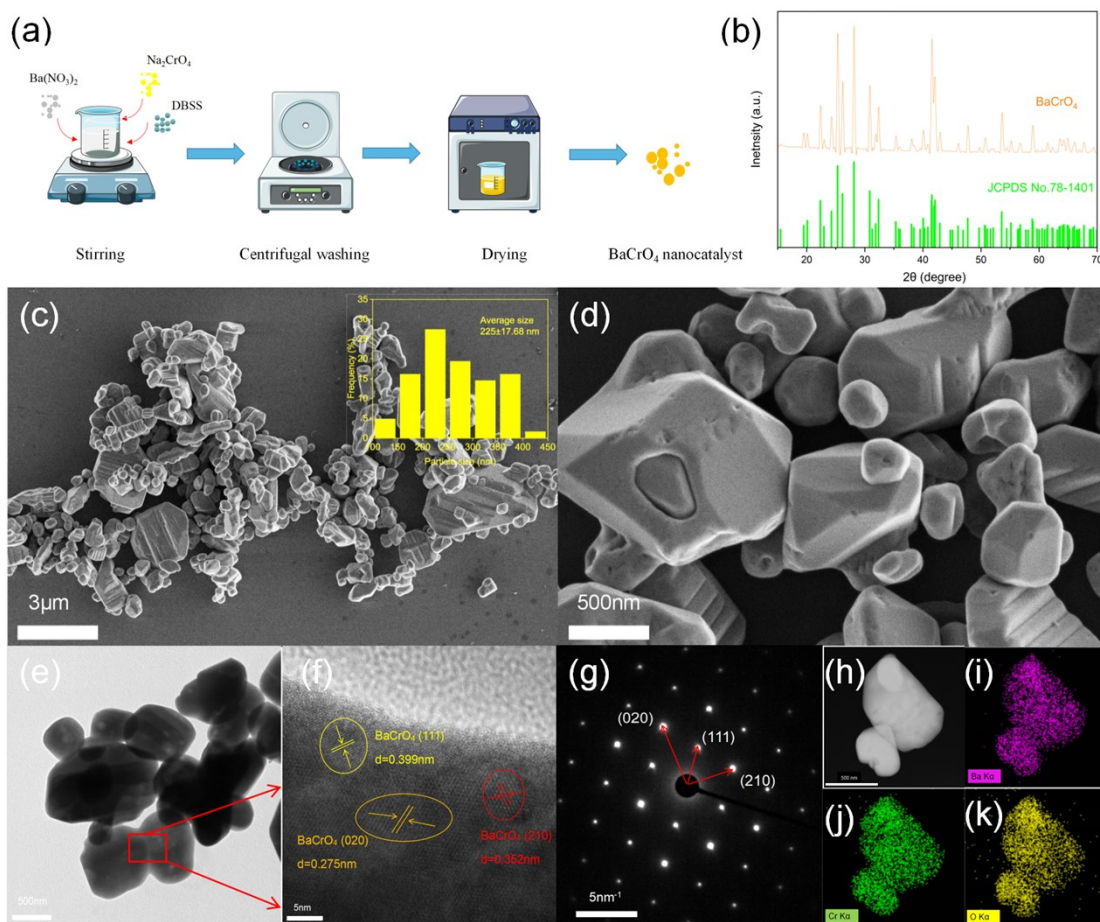


Fig. S1 (a) Preparation process of the  $\text{BaCrO}_4$  nanocatalyst, (b) XRD patterns, (c-d) SEM profiles and particle size distribution, (e-f) HRTEM image, (g) SAED image and (h-k) EDS mapping graphs of  $\text{BaCrO}_4$  nanocatalyst.

Fig S2 EDS element composition of BaCrO<sub>4</sub> nanocatalyst.

Sample	Element	Atom %
BaCrO <sub>4</sub> nanocatalyst	Ba	17.00
	Cr	13.40
	O	69.60
	Total	100

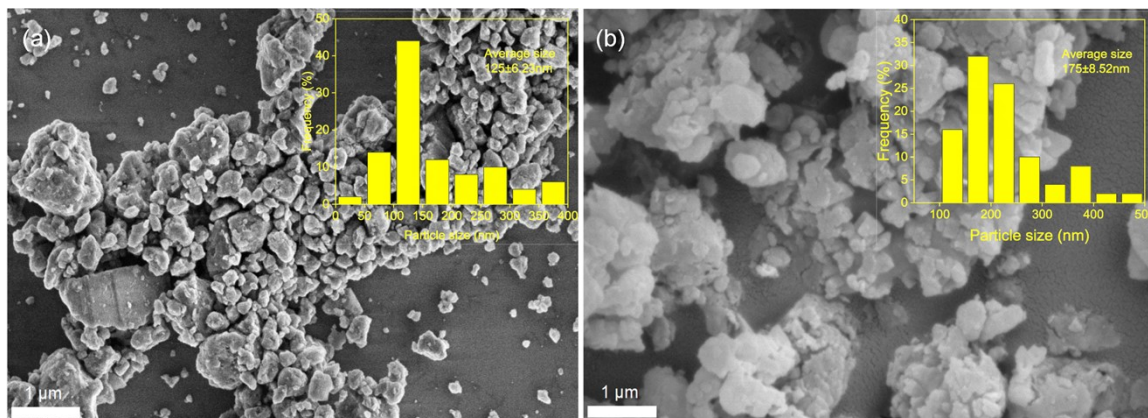


Fig. S3 SEM images and particle size distribution of (a) as-milled and (b) cycling states of 10 wt% BaCrO<sub>4</sub> introduced-MgH<sub>2</sub>.

Fig S4 EDS element composition of 10 wt% BaCrO<sub>4</sub>-introduced MgH<sub>2</sub> at different states.

Sample	Element	Atom %
10 wt% BaCrO <sub>4</sub> -introduced MgH <sub>2</sub> after milling	Ba	1.00
	Cr	0.70
	O	11.50
	Mg	86.80
	Total	100
10 wt% BaCrO <sub>4</sub> -introduced MgH <sub>2</sub> after dehydrogenation	Ba	0.88
	Cr	0.71
	O	30.24
	Mg	68.17
	Total	100
10 wt% BaCrO <sub>4</sub> -introduced MgH <sub>2</sub> after rehydrogenation	Ba	0.96
	Cr	1.13
	O	19.05
	Mg	78.86
	Total	100

Table S1 Bond length analysis of MgH<sub>2</sub> and 10 wt% BaCrO<sub>4</sub>-introduced MgH<sub>2</sub>.

Material	Average bond length of Mg-H
MgH <sub>2</sub>	1.935 Å
10 wt% BaCrO <sub>4</sub> -introduced MgH <sub>2</sub>	2.904 Å