Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2020

Supplementary Information

Ni, Beyond Thermodynamic Tuning, Maintains the Catalytic Activity of V Species in $Ni_3(VO_4)_2$ Doped MgH_2

Jiahe Zang,[a] Shaofei Wang,[bcd] Rongrun Hu,[a] Han Man,[a] Jichao Zhang,[e] Fei Wang,[a] Dalin Sun,[a] Yun Song,[a,] Fang Fang[a,*]*

[a] Department of Materials Science, Fudan University, Shanghai, 200433, PR China

[b] Institute of High Energy Physics, Chinese Academy of Sciences (CAS), Beijing 100049, China

[c] Spallation Neutron Source Science Center, Dongguan, 523808, China

[d] School of Nuclear Sciences and Technology, University of Chinese Academy of Sciences, Beijing, 100049, China

[e] Shanghai Synchrotron Radiation Facility, Zhangjiang Laboratory, Shanghai Advanced Research Institute, Chinese Academy of Sciences, Shanghai, 201204, PR China

[*]Corresponding author at: Department of Materials Science, Fudan University, Shanghai 200433 (P. R. China)

E-mail addresses: songyun@fudan.edu.cn; f_fang@fudan.edu.cn.

Content:

Table S1-S2

Table S1 Structural parameters and phase abundance for as-prepared $Ni_3(VO_4)_2$.

Sample	Space Group	Lattice parameters (Å)			Abundance
		a	*b*	*c*	
as-prepared $Ni_3(VO_4)_2$	*Cmca*	6.0157(2)	11.4295(1)	8.4315(5)	100 wt%

Table S2 Atomic coordinates, occupation factors and isotropic thermal parameters of $Ni_3(VO_4)_2$.

Atom	Site	*g*	*x*	*y*	*z*	*B* (Å^2)
Ni(1)	4*a*	1	0	0	0	0.42(3)
Ni(2)	8*e*	1	0.25	0.125	0.25	0.58(1)
V(1)	8*f*	1	0	0.4106	0.1213	0.67(3)
O(1)	8*f*	1	0	0.2292	0.2805	0.45(2)
O(2)	8*f*	1	0	0	0.2742	0.85(1)
O(3)	16*g*	1	0.2221	0.1091	0.8478	0.66(3)

Figure S1

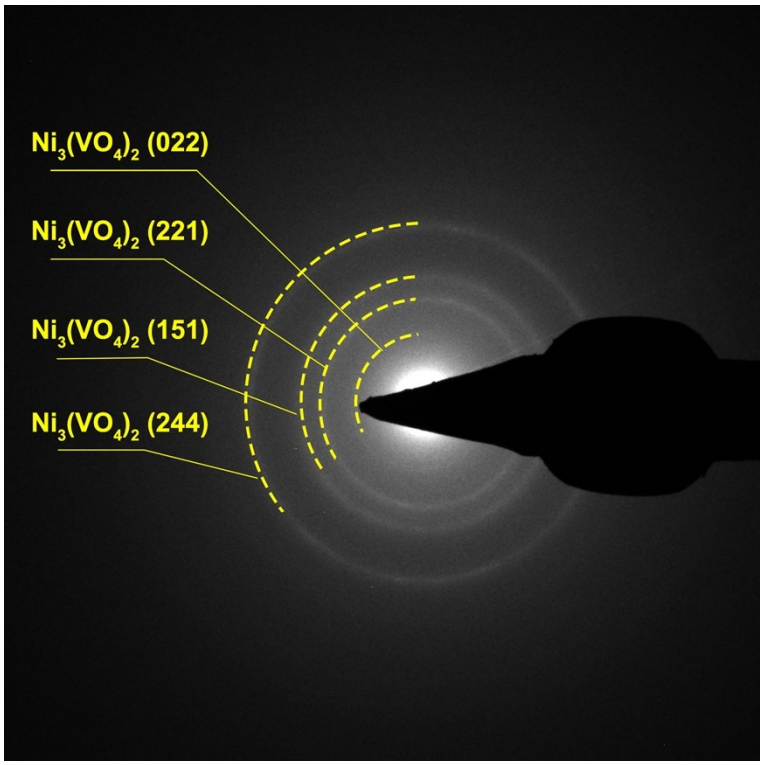

Fig.S1 Selected area electron diffraction patterns of $Ni_3(VO_4)_2$.

Figure S2

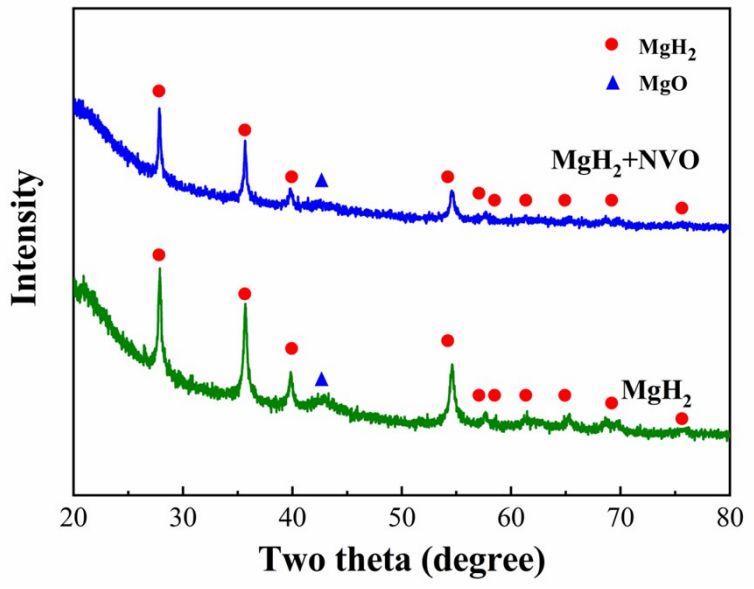

Fig.S2 XRD patterns of MgH_2-$Ni_3(VO_4)_2$ and pure MgH_2 after ball-milling.

Van't Hoff equation

The relationship between equilibrium pressures and reaction temperatures can be described by the Van't Hoff equation:

$$\ln P_{\mathrm{H_2}} = \frac{\Delta \mathrm{H}}{\mathrm{R}T} - \frac{\Delta \mathrm{S}}{\mathrm{R}} \qquad \textbf{Equation S1}$$

where T is the experimental temperature, P is the equilibrium pressure, and R is the gas constant.

Kissinger's equation

The relationship between the peak temperatures (T_P) and the different heating rates (β) is as follows:

$$\frac{\mathrm{d}[\ln(\beta / T_p^{\,2})]}{\mathrm{d}(1/T_p)} = -\frac{-E\mathrm{a}}{\mathrm{R}} \qquad \textbf{Equation S2}$$

where R is the gas constant. $\ln(\beta/T_p^2)$ vs.$1/T_p$ satisfies a linear relationship and the slope is -Ea/R.

Figure S3

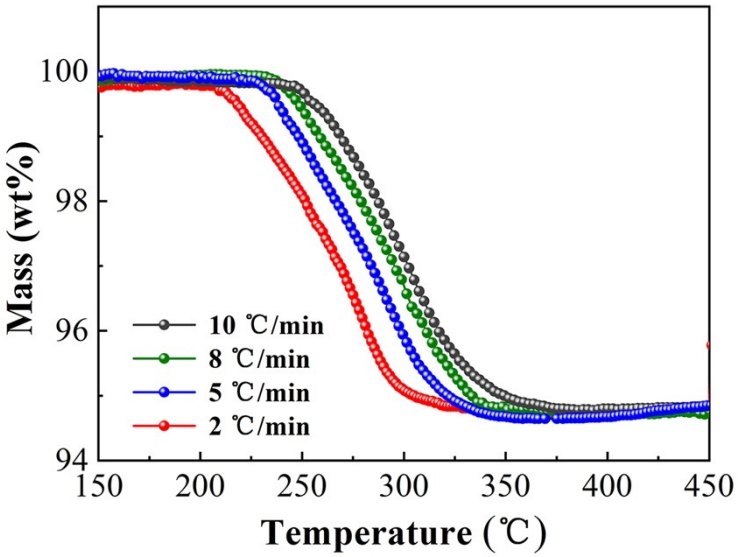

Fig.S3 TG curves of MgH_2-$Ni_3(VO_4)_2$ sample at different heating rates.

Figure S4

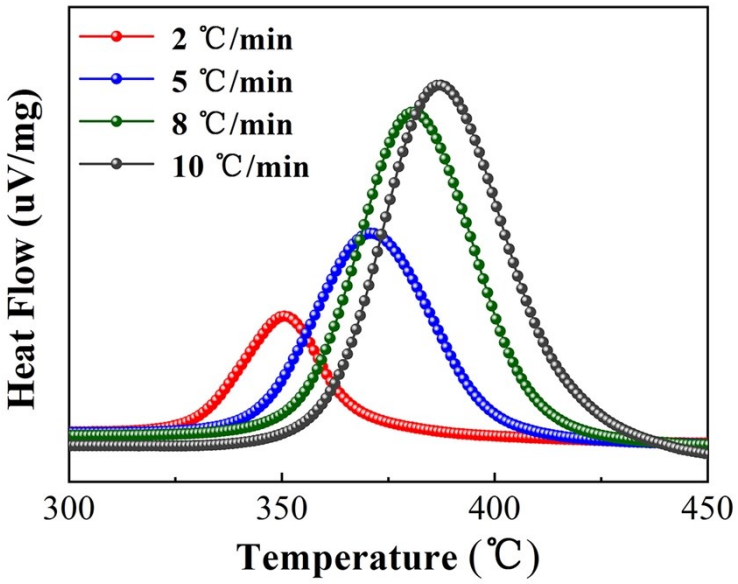

Fig.S4 DSC curves of ball-milled MgH_2 at different heating rates.

Figure S5

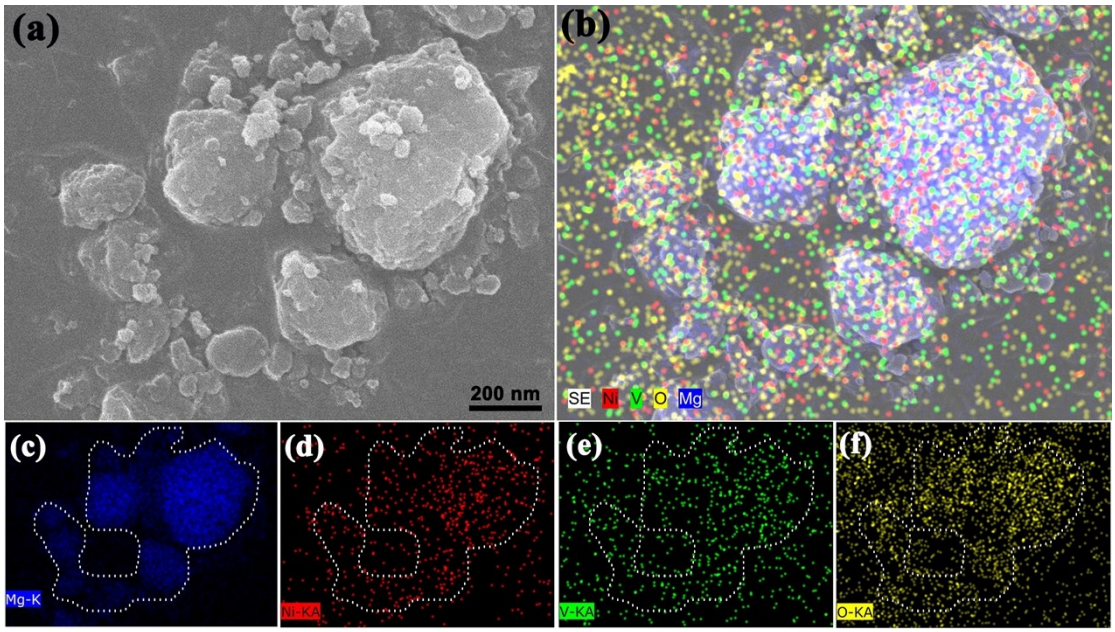

Fig.S5 (a-b) SEM, EDS mapping of (c) Mg, (d) Ni, (e) V and (f) O for dehydrogenated MgH_2-$Ni_3(VO_4)_2$ sample.

Figure S6

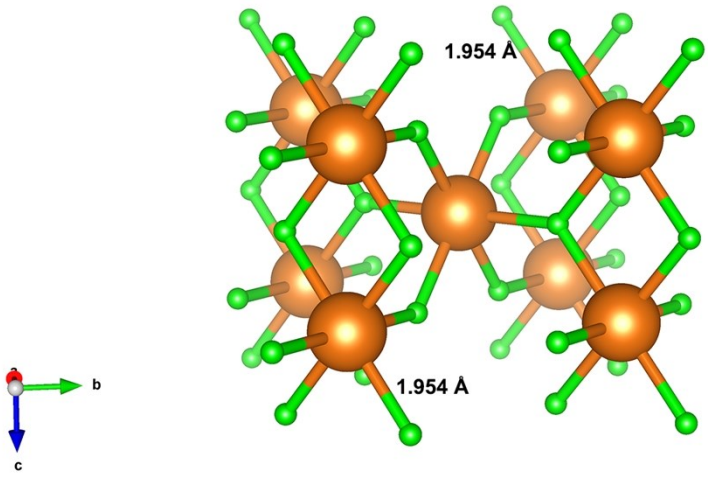

Fig.S6 Schematic diagram of the crystal structure of MgH_2.

Figure S7

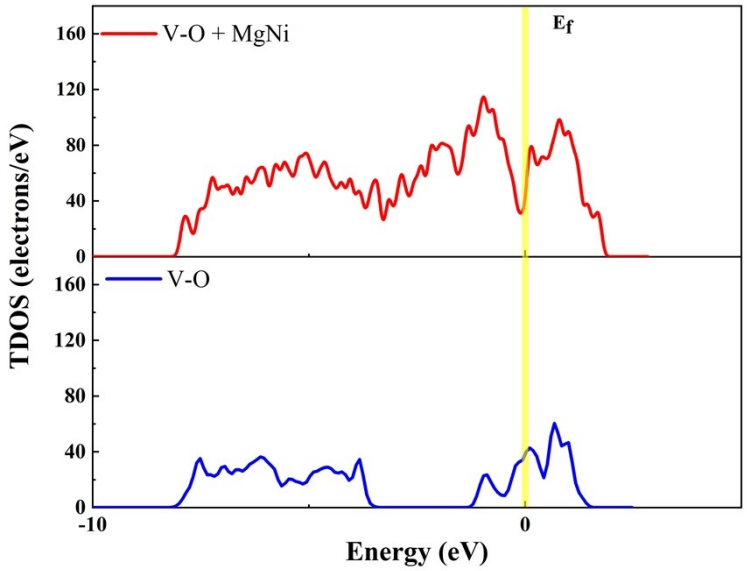

Fig.S7 DOS of V_2O_3 (001) crystal plane and Mg_2Ni doped V_2O_3.