Electronic Supplementary Information

**Vanadium oxide nanoparticles supported on cubic carbon nanoboxes as high active catalyst precursors for hydrogen storage in MgH₂†**

Zeyi Wang\(^a\), Zhuanghe Ren\(^a\), Ni Jian\(^a\), Mingxia Gao\(^a\), Jianjiang Hu\(^b\), Fang Du\(^b\), Hongge Pan\(^a\), Yongfeng Liu\(^{a,c,*}\)

\(^a\)State Key Laboratory of Silicon Materials, Key Laboratory of Advanced Materials and Applications for Batteries of Zhejiang Province and School of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, China

\(^b\)Laboratory for Energetics and Safety of Solid Propellants, Hubei Institute of Aerospace Chemotechnology, Xiangyang 441003, China

\(^c\)Key Laboratory of Advanced Energy Materials Chemistry (Ministry of Education) Nankai University, Tianjin 300071, China

\(^*\)Corresponding author

Tel/Fax: +86 571 87952615

E-mail: mselyf@zju.edu.cn
Fig. S1 Reciprocal molar magnetic susceptibility as a function of the temperature for MIL-47. Antiferromagnetic behaviour was observed below Curie temperature (50 K).

Fig. S2 N$_2$ sorption isotherm curve of the prepared nano-V$_2$O$_3$@C composite.
Fig. S3 A magnified view of XRD patterns for MgH$_2$-x wt% V$_2$O$_3$@C composites (x = 0, 9, 12) at 2θ = 28-38°.

Fig. S4 V 2p XPS spectrum of milled MgH$_2$-9 wt% V$_2$O$_3$@C sample.
Fig. S5 Dehydrogenation peak temperatures obtained in the literature compared with our result.

Fig. S6 SEM images of as-milled MgH$_2$ (a) and MgH$_2$-9 wt% V$_2$O$_3$@C (b).

Fig. S7 XRD patterns of prepared nano-V$_2$O$_3$ (a) and isothermal dehydrogenation curves of MgH$_2$ with different additives (V$_2$O$_3$@C, V$_2$O$_3$, V$_2$O$_3$/C) at 250 °C (b).
Fig. S8 Isothermal hydrogenation curves of the milled MgH₂.

Fig. S9 TPD curves of MgH₂-9 wt% V₂O₅@C at different heating rates.
**Fig. S10** Comparison of dehydrogenation curves of MgH$_2$ added with 9 wt% and 20 wt% V$_2$O$_3$@C.

**Fig. S11** A magnified view of XRD patterns for MgH$_2$-20 wt% V$_2$O$_3$@C sample at different dehydrogenation stages.
Fig. S12 HRTEM image of dehydrogenated MgH$_2$-20 wt% V$_2$O$_3$@C sample.

Fig. S13 V 2p XPS spectra of MgH$_2$-20 wt% V$_2$O$_3$@C samples after the 1$^{\text{st}}$ hydrogenation (a) and 2$^{\text{nd}}$ dehydrogenation (b).