**Electronic Supplementary Information**

# Vanadium oxide nanoparticles supported on cubic carbon nanoboxes as high active catalyst precursors for hydrogen storage in $MgH_2$†

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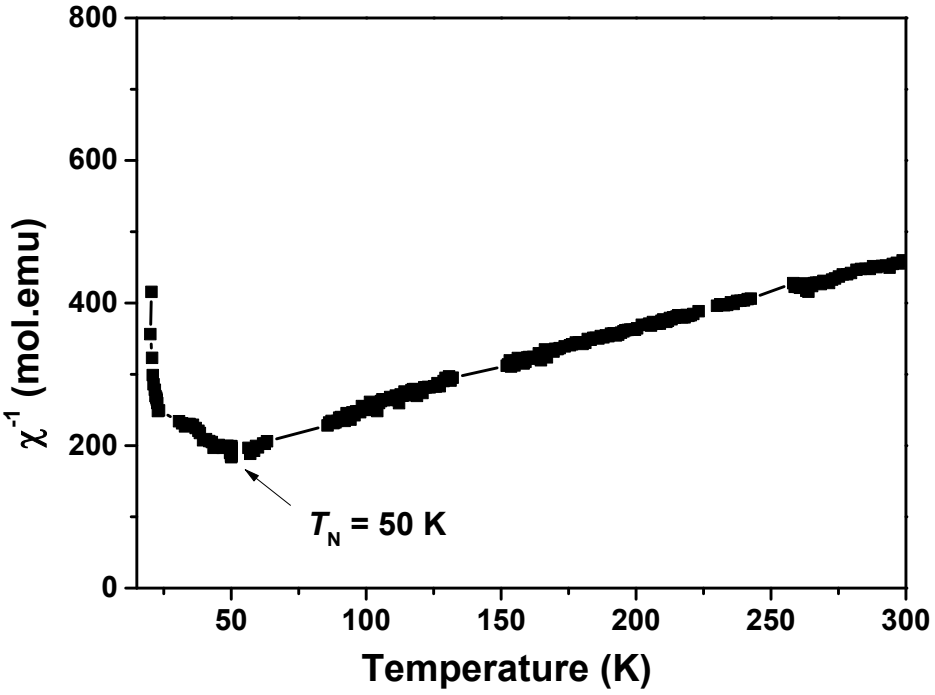


**Fig. S1** Reciprocal molar magnetic susceptibility as a function of the temperature for MIL-47. Antiferromagnetic behaviour was observed below Curie temperature (50 K).

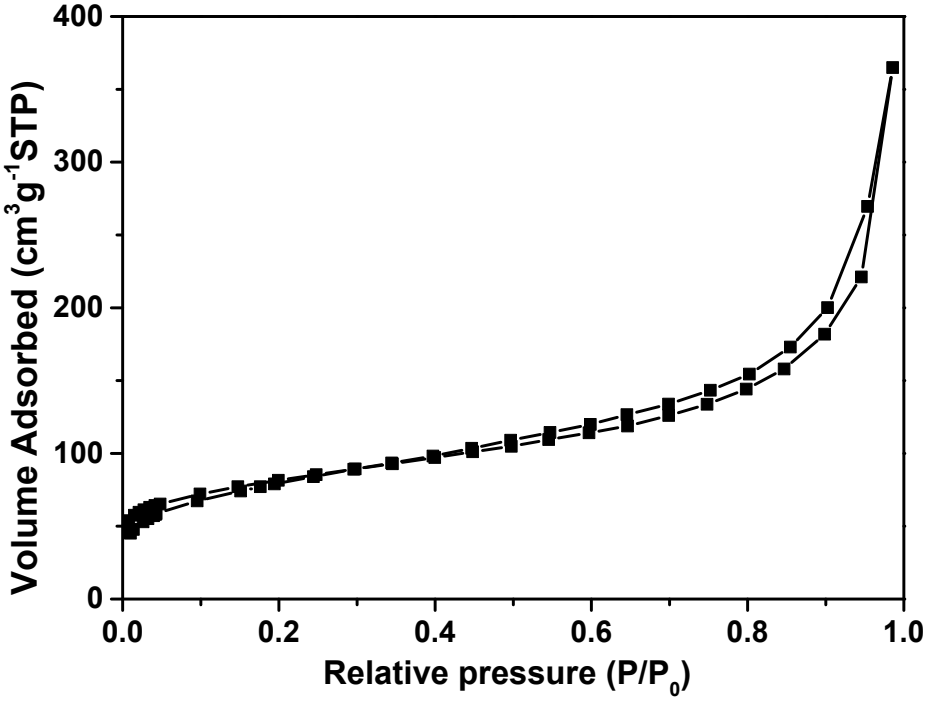


**Fig. S2** $N_2$ sorption isotherm curve of the prepared nano-$V_2O_3$@C composite.

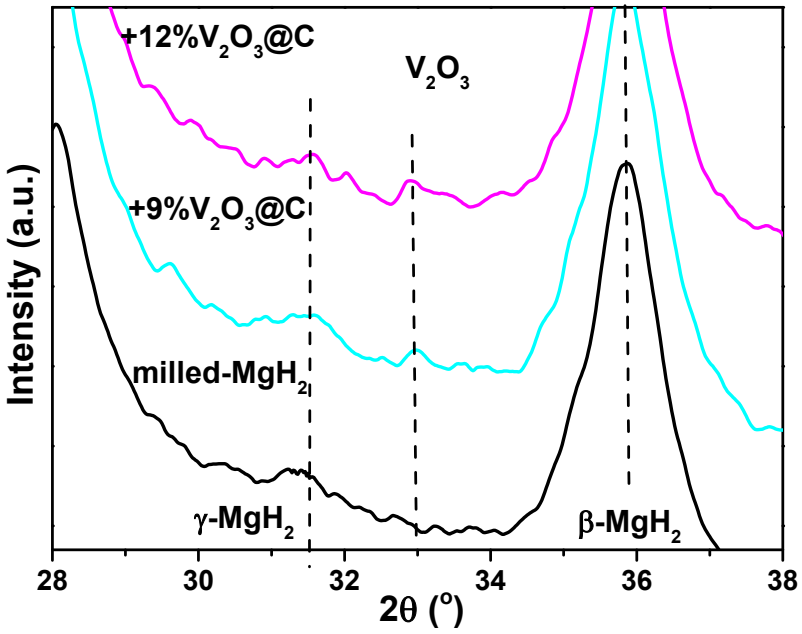


**Fig. S3** A magnified view of XRD patterns for $MgH_2$-*x* wt% $V_2O_3$@C composites (*x* = 0, 9, 12) at 2θ = 28-38°.

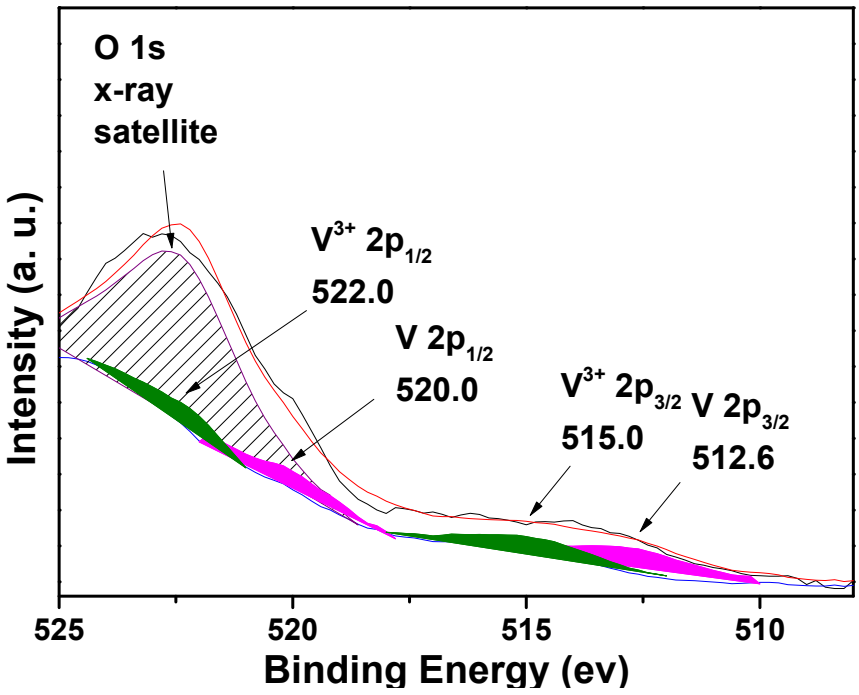


**Fig. S4** V 2p XPS spectrum of milled $MgH_2$-9 wt% $V_2O_3$@C sample.

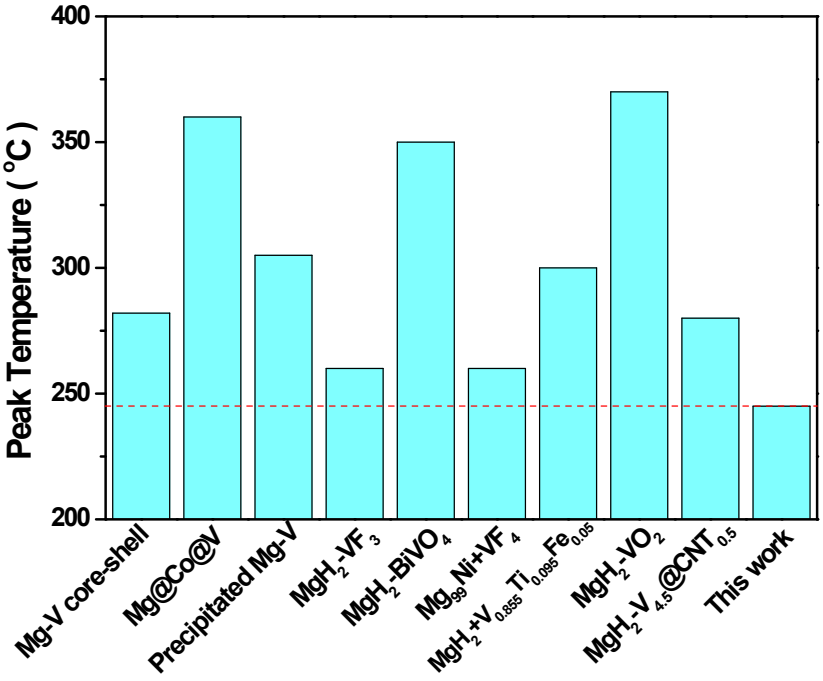


**Fig. S5** Dehydrogenation peak temperatures obtained in the literature compared with our result.

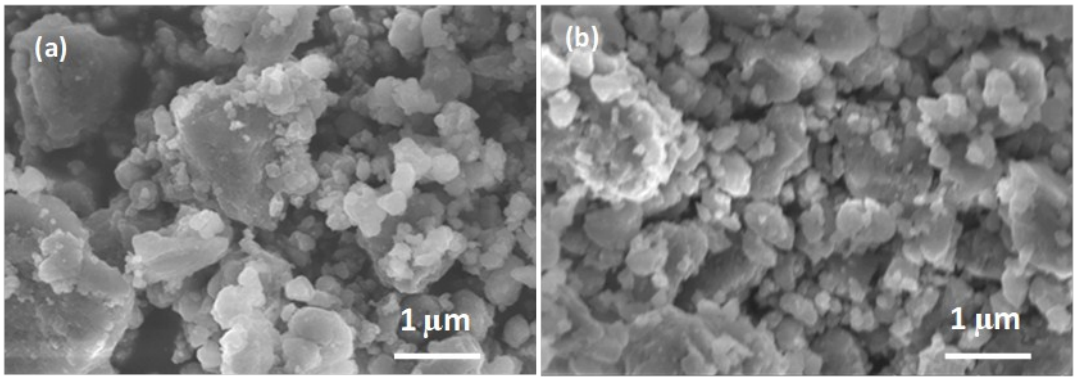


**Fig. S6** SEM images of as-milled $MgH_2$ (a) and $MgH_2$-9 wt% $V_2O_3$@C (b).

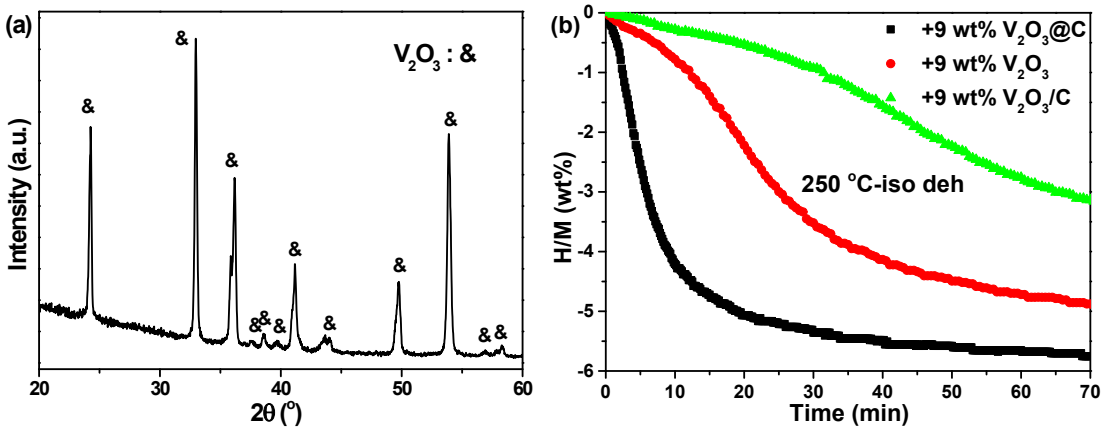


**Fig. S7** XRD patterns of prepared nano-$V_2O_3$ (a) and isothermal dehydrogenation curves of $MgH_2$ with different additives ($V_2O_3$@C, $V_2O_3$, $V_2O_3$/C) at 250 °C (b).

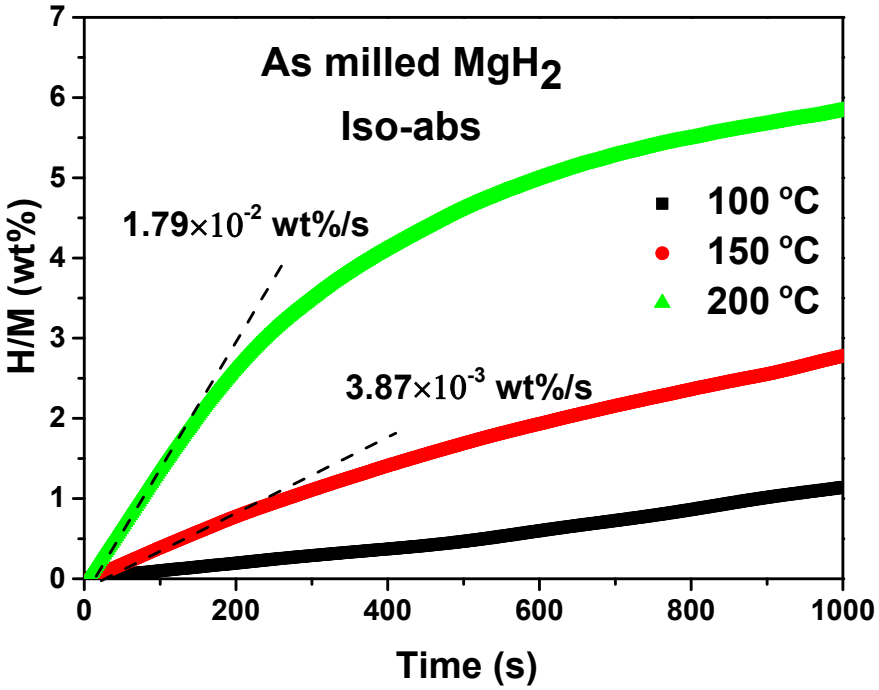


**Fig. S8** Isothermal hydrogenation curves of the milled $MgH_2$.

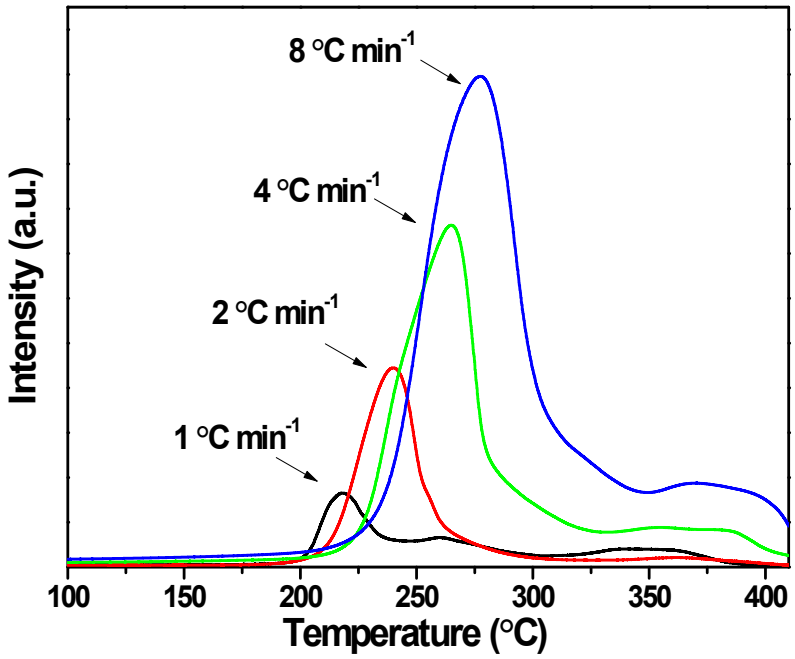


**Fig. S9** TPD curves of $MgH_2$-9 wt% $V_2O_3$@C at different heating rates.

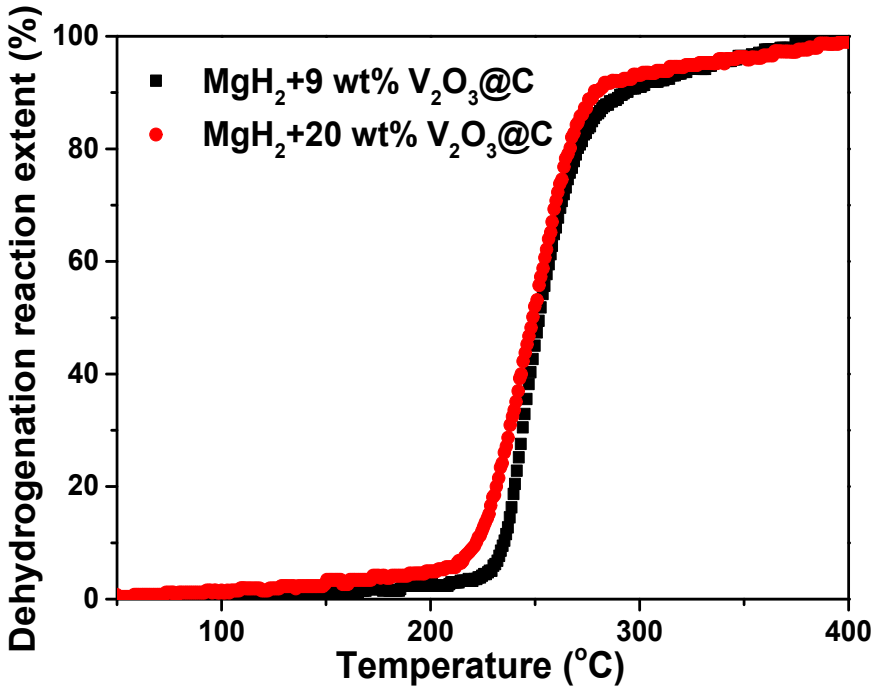


**Fig. S10** Comparison of dehydrogenation curves of $MgH_2$ added with 9 wt% and 20 wt% $V_2O_3$@C.

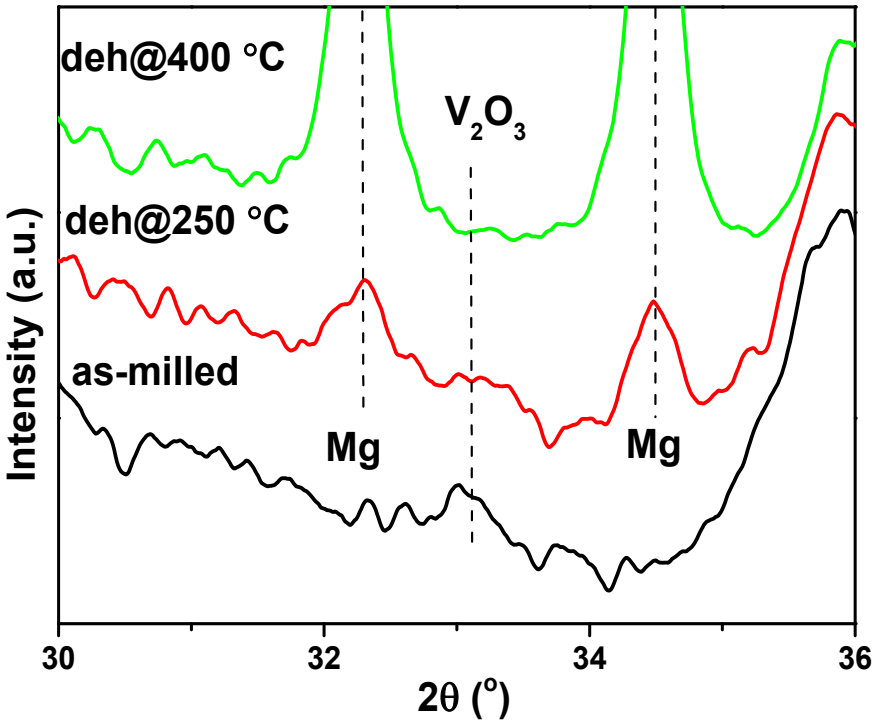


**Fig. S11** A magnified view of XRD patterns for $MgH_2$-20 wt% $V_2O_3$@C sample at different dehydrogenation stages.

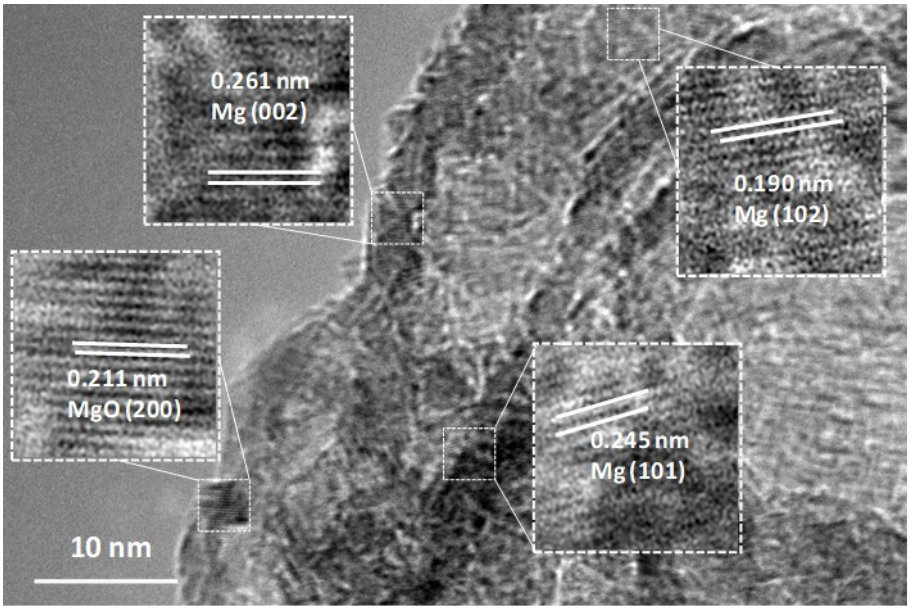


**Fig. S12** HRTEM image of dehydrogenated $MgH_2$-20 wt% $V_2O_3$@C sample.

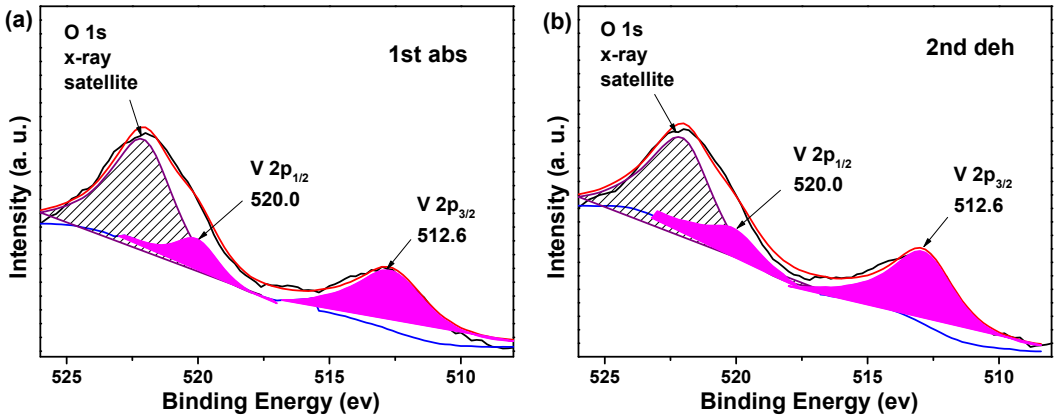


**Fig. S13** V 2p XPS spectra of $MgH_2$-20 wt% $V_2O_3$@C samples after the 1st hydrogenation (a) and 2nd dehydrogenation (b).