Structural Evolution of Reversible Mg Insertion into a Bilayer Structure of V2O5·nH2O Xerogel Material

Niya Sa,[†‡*] Tiffany L. Kinnibrugh,[#] Hao Wang,[†‡] Gopalakrishnan Sai Gautam,[§] Karena W. Chapman,[#] John T. Vaughey,[†‡] Baris Key,[†‡] Timothy T. Fister,[†] John W. Freeland,[#] Danielle L. Proffit,[†‡] Peter J. Chupas,[#] Gerbrand Ceder,[§] Javier G. Bareno,[‡] Ira D. Bloom,[‡] Anthony K. Burrell[†‡*]

[†]Joint Center for Energy Storage Research, Argonne National Laboratory, Lemont, IL 60439, USA
[‡]Chemical Science and Engineering Division, Argonne National Laboratory, Lemont, IL 60439, USA
[#]X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439, USA
[§]Material Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

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TGA analysis: Thermogravimetric analysis (TGA) of the pristine $V_2O_5 \cdot nH_2O$ xerogel was conducted on a Perkin Elmer Pyris Instrument inside of an argon-filled glove box with H_2O and O_2 level less than 1 ppm. The weight change profile was characterized by a steep loss program before 80 °C, followed with a gradual weight loss program with 3 °C /min increase of temperature till 800 °C. Figure S1 showed weight loss profile that is composed of two parts, the first slope observed for weight loss before 150 °C which corresponds to weakly bound water and the second slope corresponds to tightly bound water.

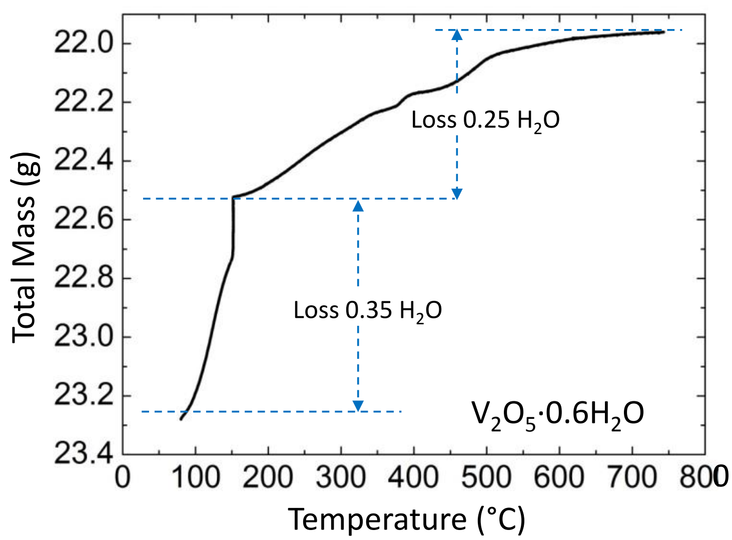

Figure S1. Thermogravimetric analysis (TGA) curves for pristine $V_2O_5 \cdot nH_2O$ xerogel sample. Weight loss corresponding to weakly bond water (T < 150 °C) and tightly bond water (T > 150 °C) is shown.

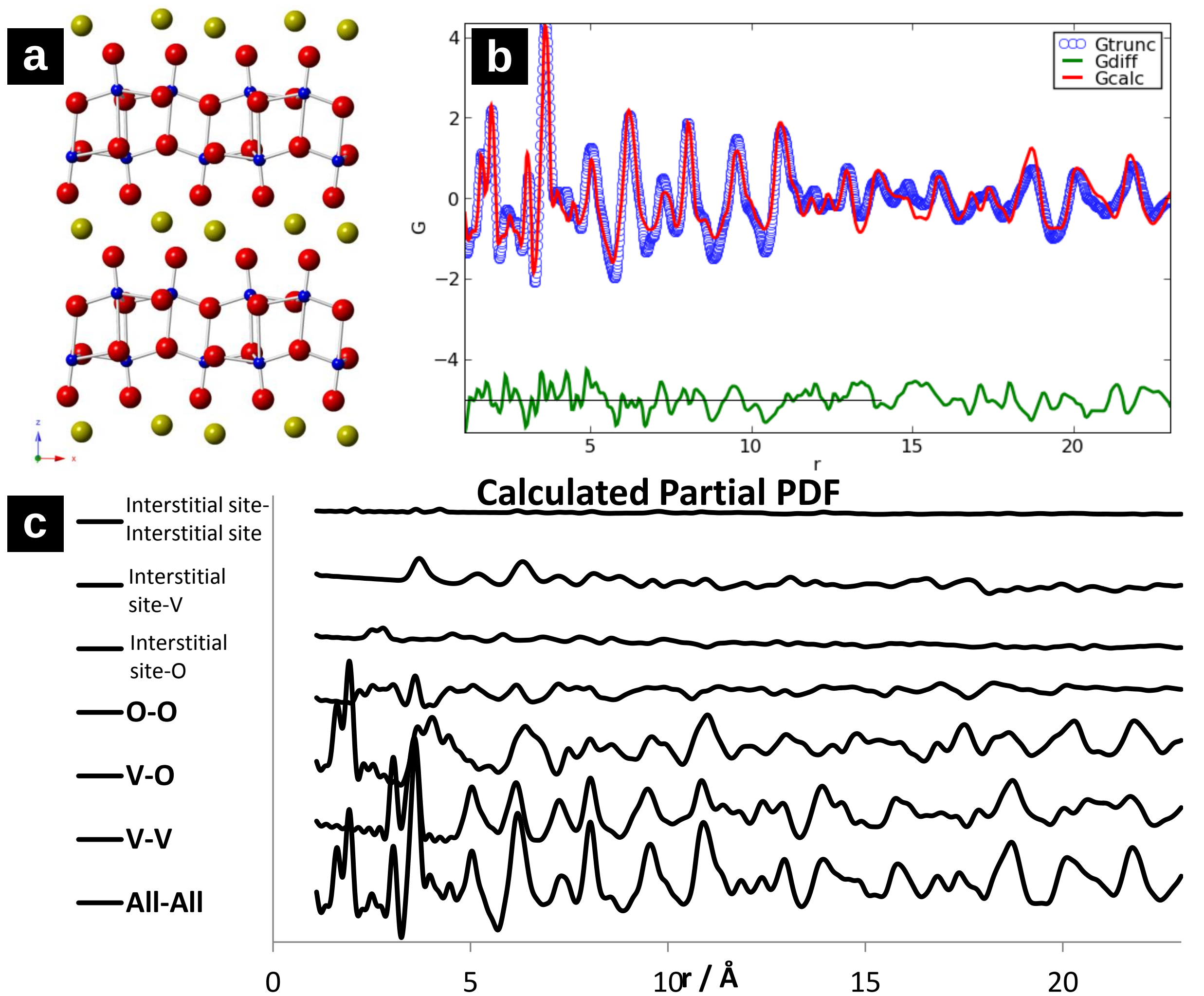

Figure S2. Pair distribution function (PDF) analysis for xerogel $V_2O_5{\cdot}nH_2O$. Structure model is based on $V_2O_5{\cdot}nH_2O$ with interstitial species. **(a)**. Double layer structure of xerogel $V_2O_5{\cdot}nH_2O$, where red, yellow and blue stand for oxygen, water molecules and vanadium, respectively. **(b)**. Experimental (hollow blue line) and calculated PDF (solid red line) for $V_2O_5{\cdot}nH_2O$ xerogel. **(c)**. Calculated partial PDF for Interstitial site-interstitial site, Interstitial site-V, Interstitial site-O, O-O, V-O, V-V over 20 Å.

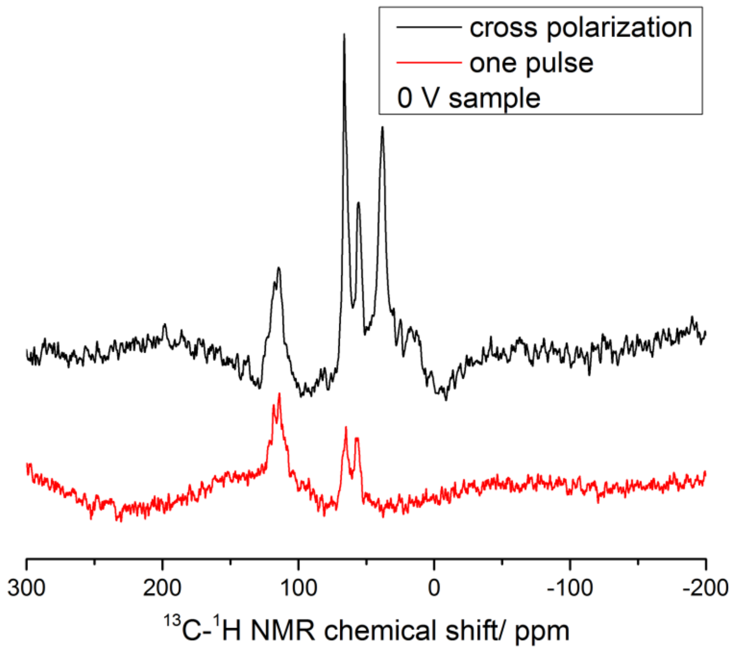

Figure S3. ^{13}C NMR spectra of discharged sample (0 V). black: one pulse experiment, red: ^{1}H-^{13}C cross polarization experiment.

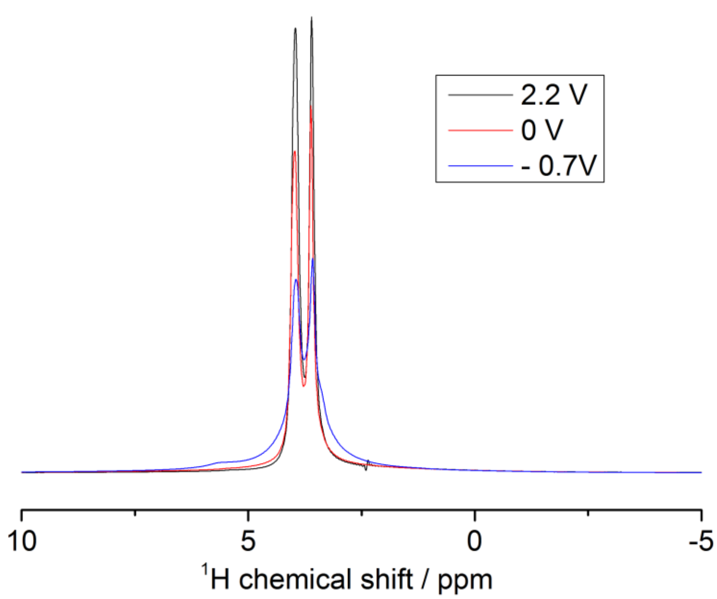

Figure S4: ^{1}H NMR spectra of a secondary set of charged/discharged sample.

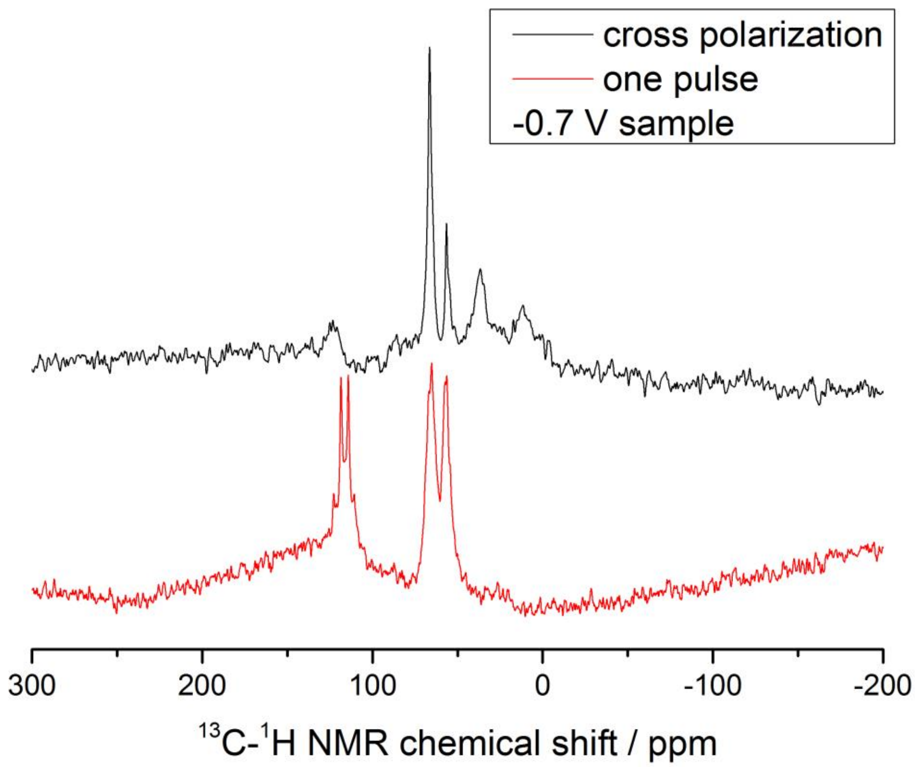

Figure S5. ^{13}C NMR spectra of the -0.7 V sample in Figure S4. Black: ^{1}H-^{13}C cross polarization experiment, red: one pulse experiment.

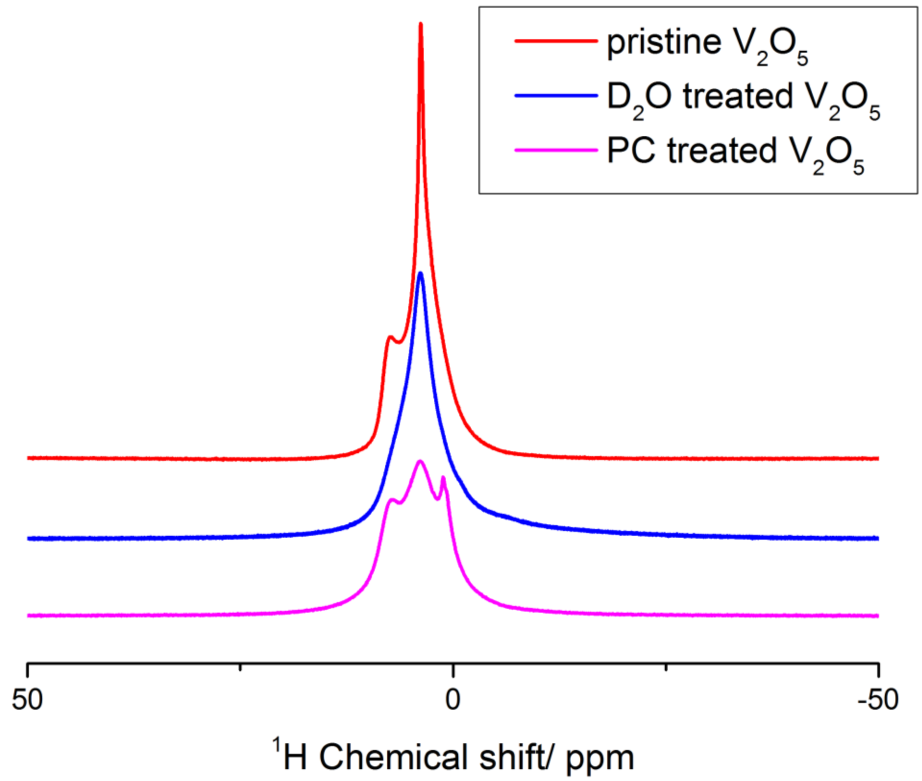

Figure S6. ^{1}H NMR spectra of pristine V_2O_5, D_2O treated V_2O_5 and PC treated V_2O_5.

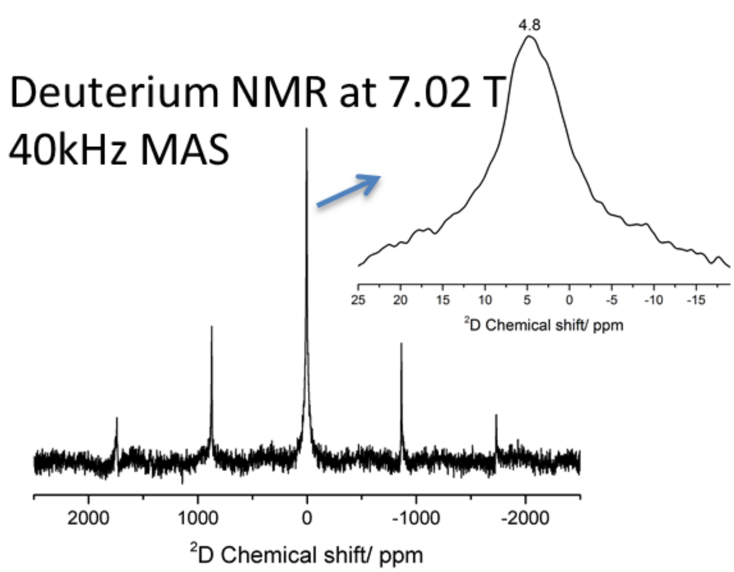

Figure S7. ^{2}H NMR spectra of D_2O treated V_2O_5

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