

SUPPLEMENTARY INFORMATION

Temperature-resolved nanoscale hydration of a layered manganese oxide

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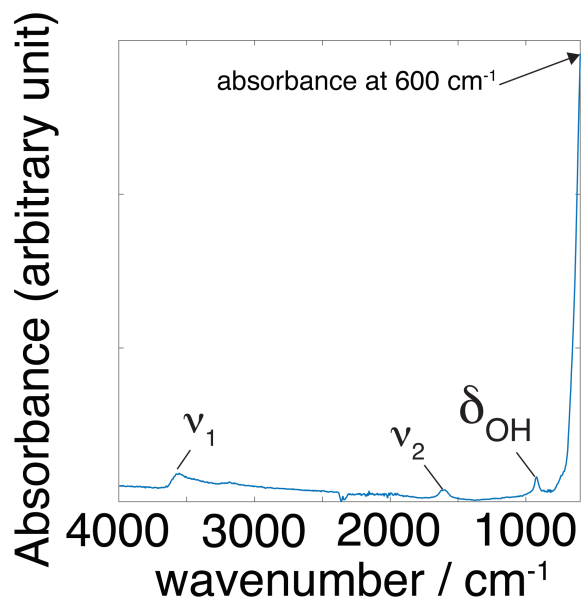


Fig. S1. FTIR spectrum of birnessite dried under $N_2(g)$ for 24 h, also showing residual water (ν_1 , ν_2). Absorbance values of dry at 600 cm^{-1} prior exposure to water were used to normalize all spectra.

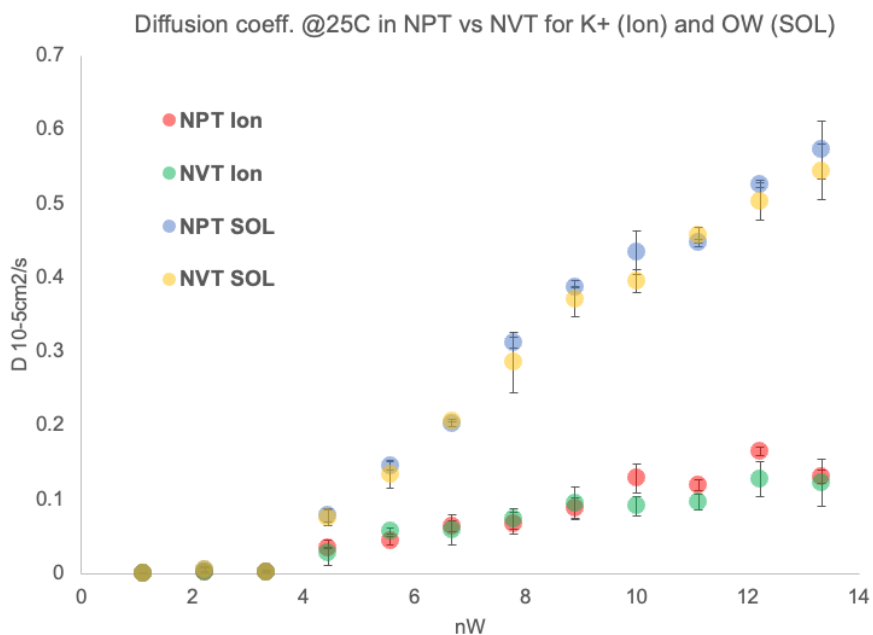


Fig. S2 Comparison of K^+ (Ion) and water (SOL) diffusion coefficients obtained by simulations run under isobaric-isothermal (NPT) and canonical (NVT) ensembles.

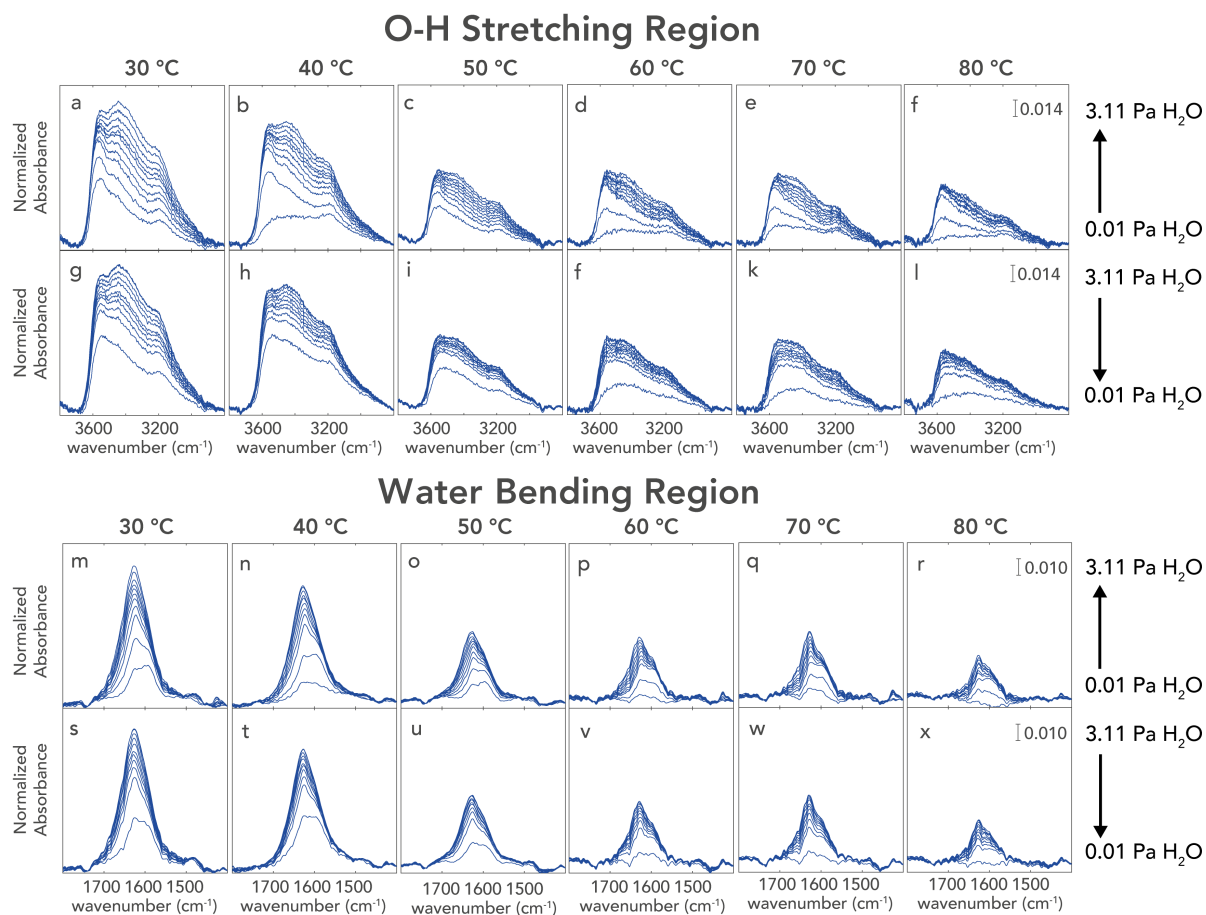


Fig. S3. FTIR spectra of birnessite exposed to a 500 mL/min flow flow 0-3.11 kPa H₂O in N₂(g) (total pressure of 101 kPa) during (a-f, m-r) adsorption (Fig. 2 of main text) and (g-l, s-x) desorption legs at (a, g, m, s) 30, (b, h, n, t) 40, (c, i, o, u) 50, (d, f, p, v) 60, (e, k, q, w) 70, and (f, l, r, x) 80 °C. All absorbances were normalised for the quantity of MnO₂ based on the intensity of the Mn-O stretching band at 600 cm⁻¹ (Fig. S1).

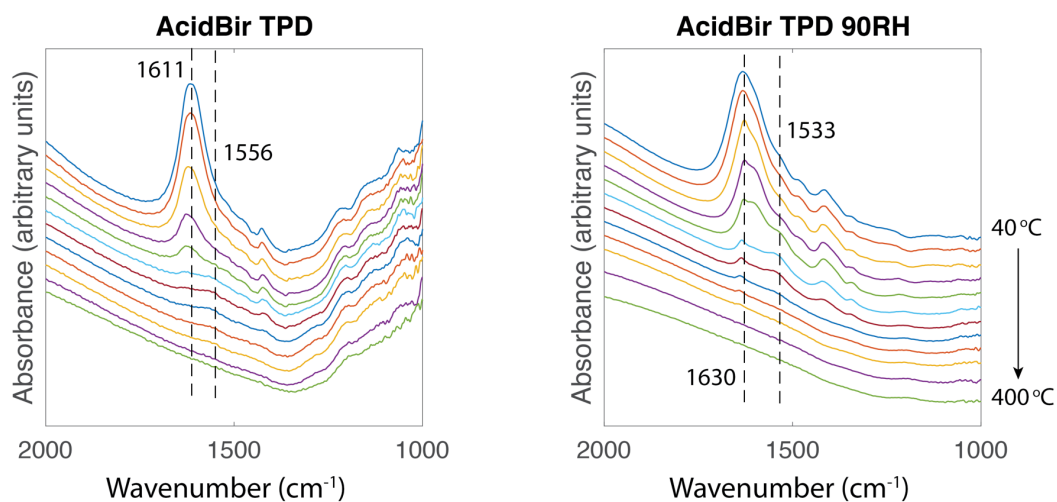


Fig. S5. Temperature programmed desorption (TPD) experiment of acid birnessite heated up to 400 °C at a gradient of 10 °C/min (left) under vacuum and (right) under a flow of 500 mL/min N₂(g) with 90% RH (3.11 kPa H₂O).

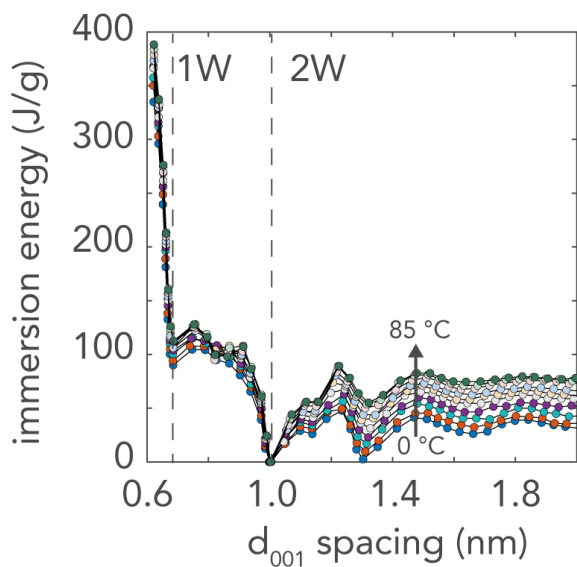


Fig. S6. Predicted immersion energy profiles versus d₀₀₁-spacing, showing the 1W state at 1.33 H₂O/UC (5.33 H₂O/K⁺; d₀₀₁-spacing=0.685 nm) and the 2W state at 3.33 H₂O/UC (13.33 H₂O/K⁺; d₀₀₁-spacing=1.00 nm).

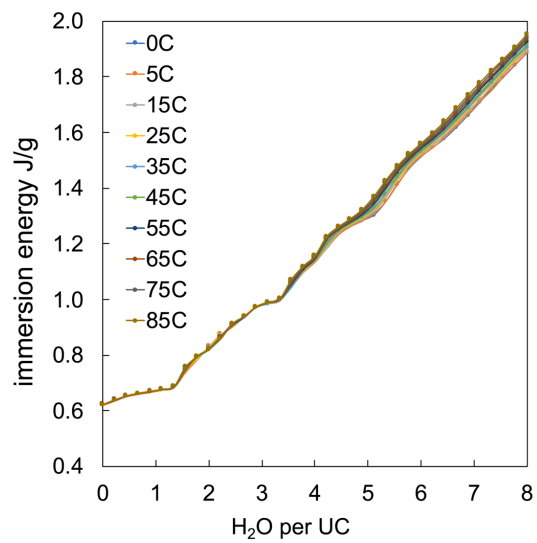


Fig. S7. Predicted immersion energy profiles versus water per unit cell (UC).