

Supplementary Information For

**Sensing of NO₂ with Zirconium Hydroxide via Frequency-
Dependent Electrical Impedance Spectroscopy**

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ATR-FTIR

Figure S1 shows a schematic of the system used to expose the samples to NO₂ gas. The BET surface area and pore volume for the samples are reported in Table S1. After various concentrations of NO₂ gas exposure, ATR-FTIR spectra were collected to confirm adsorption of NO₂ on Zr(OH)₄ using a Bruker Tensor 27 FTIR with a platinum accessory and a single reflection diamond crystal. An average of sixteen scans from 400-2000 cm⁻¹ with background subtraction was collected. The instrument resolution was 4 cm⁻¹. Samples were evaluated on unexposed and nitrogen dioxide exposed. As shown in Figure S2, there are asymmetrical and symmetrical N–O vibrational stretches in the 1550 and 1365 cm⁻¹ regions, respectively, and the asymmetric stretch of N–O at 1530 cm⁻¹ is observed more clearly at 1000 ppm than at lower concentrations of NO₂. These results support adsorption of NO₂ on the surface. Other unspecified peaks in the fingerprint region are intrinsic to the Zr(OH)₄, e.g. Zr–O and some weak O–H stretches.

Material	BET Surface Area (m²/g)	Pore Volume (cc/g)
Zr(OH) ₄ powder	407	0.81
Zr(OH) ₄ Pressed @ 5 kpsi	390	0.68
Zr(OH) ₄ exposed to 1000 ppm NO ₂	309	0.55

Table S1. BET surface area and pore volume for samples after pressing and exposure to nitrogen dioxide.

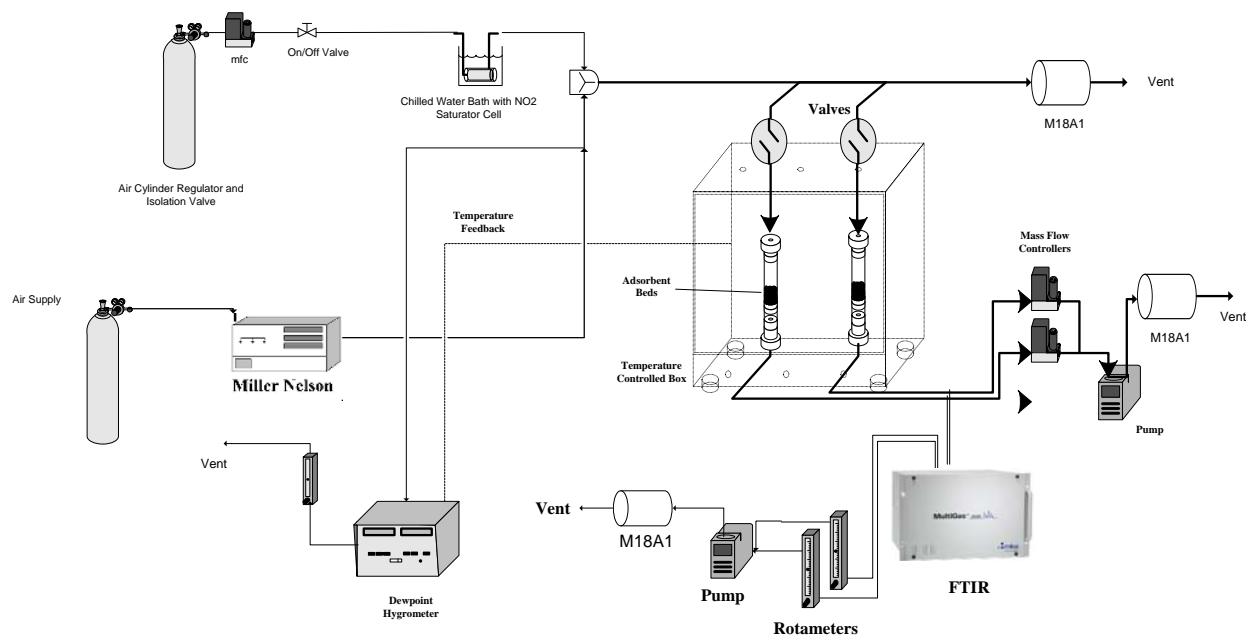


Figure S1. Schematic of the system and dosing setup.

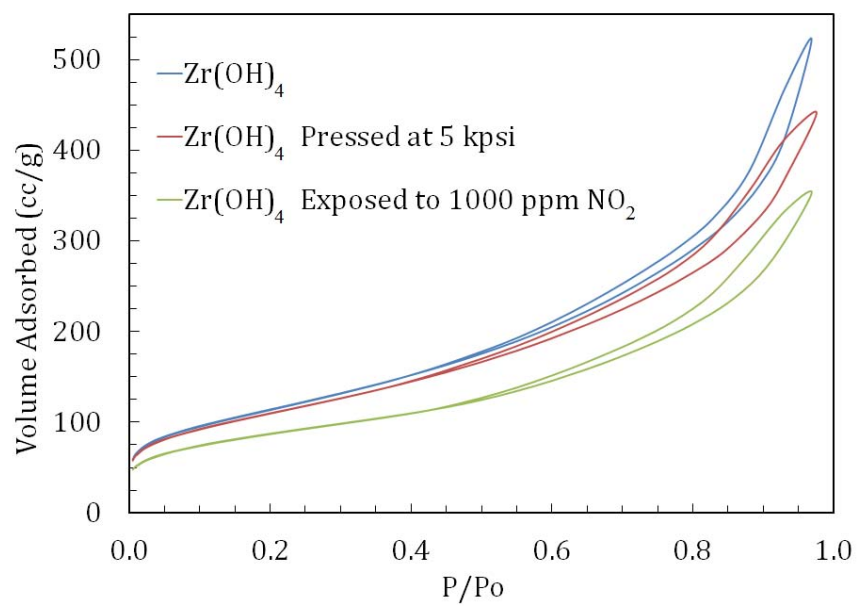


Figure S2. Nitrogen isotherm data for zirconium hydroxide after pressing and exposure to nitrogen dioxide.

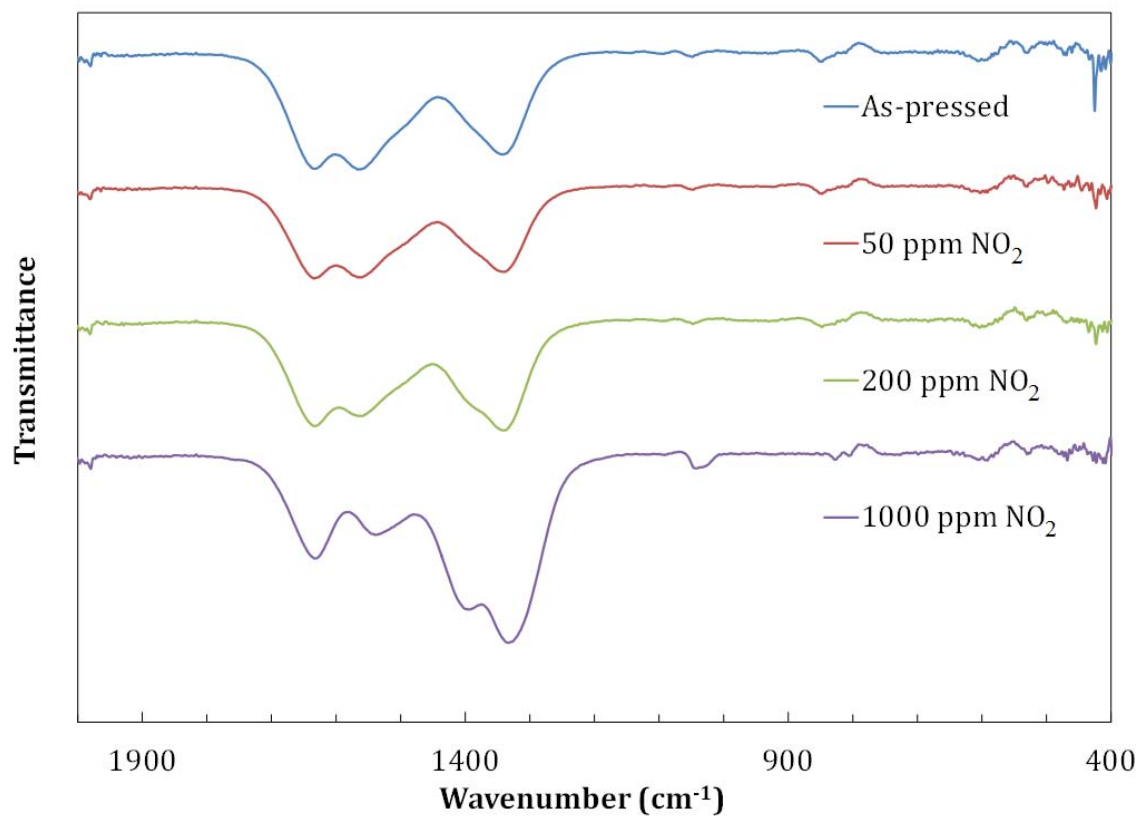


Figure S3. Waterfall plot of attenuated total reflectance Fourier infrared spectra for Zr(OH)₄ (blue) and Zr(OH)₄ exposed to 50 (red), 200 (green), and 1000 ppm·h (purple) of NO₂.

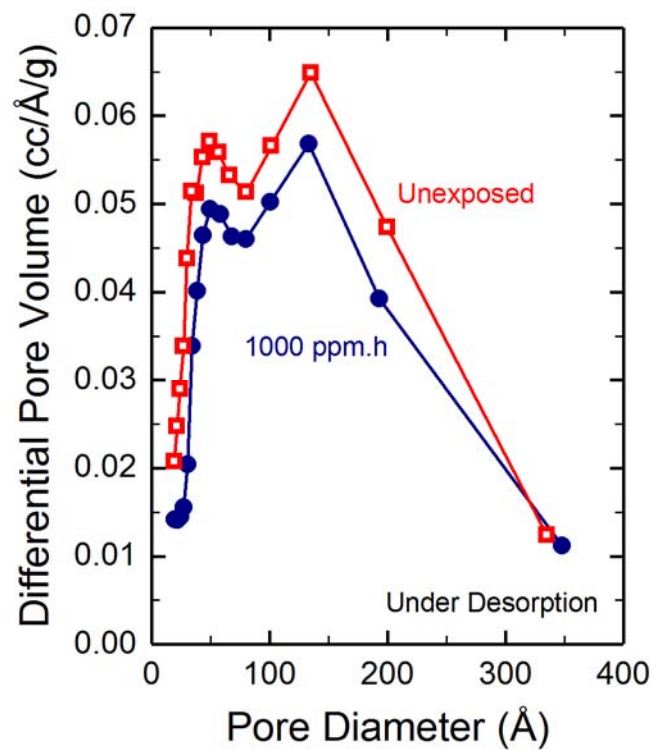


Figure S4. Differential pore size distributions (pore volume as a function of pore diameter) under N₂ desorption for unexposed Zr(OH)₄ (open red squares) and Zr(OH)₄ exposed to 1000 ppm·h dose (solid blue circles) of NO₂.